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Appendices

Appendix A: Matlab® Program

An Example of the M-file Script Routines Used to Calculate the Electron and the Hole Wavefunctions for Multiple Quantum Dots by Solving the Schrödinger Equation Using the Different Effective Masses Approach

The whole calculation program is divided into three files:

PD_BI_QDs.m -- the main routine used to calculate polarization degree of bi-QDs

Call-BIQDs.m -- the subroutine called to define the region of InAs and GaAs

BiQD_eigenergy.m -- the subroutine called to calculate the eigen-energies and eigen-functions of QDs

List of the routines:

PD_BI_QDs.m

```
clc
clear
close all
clear all

  x0 = 0; xf=120;       % starting and end points of x axis (in units of nanometers)
  y0 = 0; yf=120;       % starting and end points of y axis (in units of nanometers)
  Mx =60;               % Number of sample points in x axis (in units of nanometers)
  My =60;
  dx = (xf - x0)/Mx;
  dy = (yf - y0)/My;
   x = (-xf/2:xf/Mx:xf/2);    %position of sample points in x axis
   y = (-yf/2:yf/Mx:yf/2)';   %position of sample points in y axis

% NUMERICAL CALCULATION of the Schroedinger equation implemented by using Finite
% Difference Method
% Developed by Nan Thidar Chit Swe
% The maximum mesh size for the two-dimensional Schroedinger equation is 60*60.
% One mesh is equivalent to 2 nm.
%-------------------------------------------------------------------
%-------------------------------------------------------------------

% Calculate the electron wavefunction
 disp( '%This program shows the wavefunctions obtained by solving the Schroedinger')
 disp('equation for BINARY quantum dots. The size of the dot is fixed at 20 nm.')
 disp ('%')
 disp( '%Calculating the electron wavefunction')
 disp ('%')
```

```
disp(' %The value of the band offset V1 is 0.31 eV.')
disp ('%')
disp('%The length in the x direction and the y direction each is 120 nm.')
disp ('%')
disp('%The number of the mesh points in the x and x directions is 60 each.')
disp ('%')
disp(' %This program calculates based on the interdot spacing between QDs.')
disp ('%')
disp('Distance between QDs: 2d'  );
disp ('%')
d=input ('d=');
num_sol=input ('%number of solutions:       ');
disp ('%')
m1=input ('%mass of electron in GaAs:       ');
m2=input('%mass of electron in InAs:       ');
disp ('%')
disp ('%')
Vp=input ('%band offset (eV):       ');

[phi,te,d,num_sol,V1,V]=BiQD_eigenergy(d,num_sol,Mx,My,Vp,m1,m2);

 figure(1);

 mesh(x,y,V1)
  xlabel('Distance (nm)')
  ylabel('Distance (nm)')
  zlabel('Potential energy, (eV)')

   A= reshape(phi(:,1),Mx-1,My-1);
   Phielectron=zeros(Mx+1,My+1);
   Phielectron(2:Mx,2:end-1)=A(1:end,1:end);
    Xlabel ('X-Distance (nm)'),
    ylabel ('Y-Distance (nm)')'
    zlabel ('Wavefunction');
    title  ('Electron wavefunction of the QDs')
    figure(2);
    mesh(x,y,Phielectron)
   %-----------------------------------------------------------------
   %-----------------------------------------------------------------

% Calculate the hole wavefunction
m1=input ('%mass of hole in GaAs:       ');
m2=input('%mass of hole in  InAs:       ');
[phi,te,d,num_sol,V,V1]=BiQD_eigenergy(d,num_sol,Mx,My,Vp,m1,m2);

    figure(3);
    mesh(x,y,V)
    xlabel('Distance (nm)')
    ylabel('Distance (nm)')
    zlabel('Potential energy, (eV)')
```

```
B= reshape(phi(:,1),Mx-1,My-1);
   Phihole=zeros(Mx+1,My+1);
   Phihole(2:Mx,2:end-1)=B(1:end,1:end);

   figure(4);
   mesh(x,y,Phihole);
   xlabel('X-Distance (nm)'),
   ylabel('Y-Distance (nm)')'
   zlabel('Wavefunction');
   title('Figure (4) : Hole wavefunction of the QDs')
  %-------------------------------------------------------------------
  %-------------------------------------------------------------------

% Calculate the overlap integral
  Phi1=Phihole.*Phielectron;
  A = sum(sum(Phi1(25:My-25+1,30-n+1:30+n+1)))
  Area = (10*2*n)
  overlap= A/Area
  %------------------------------------------------------------------
  %------------------------------------------------------------------

% Calculate the Linear Polarization Degree (PD)
    [X,Y]=meshgrid(x,y);
    D1=abs(Phielectron.*X.* Phihole);
    D2=abs(Phielectron.*Y.* Phihole);
    A=((dx*dy)/4)*1/4* (sum (sum(D1(2:Mx,2:end-1))));
    B=((dx*dy)/4)*1/4* (sum (sum(D2(2:Mx,2:end-1))));
    C=overlap*((A-B)/(B+A))
```

Call-BIQDs.m

```
function[mass,V1,V,const]=call_BiQD(d,Vp,m1,m2,Mx,My);

 x0 = 0; xf=120;        % starting and end points of x axis (in nanometers)
 y0 = 0; yf=120;        % starting and end points of y axis (in nanometers)

 dx = (xf - x0)/Mx;      % increment in x direction = length(nm)/Mx
 x = x0 + [0:Mx]*dx;     % position of sample points in x direction
 dy = (yf - y0)/My;      % increment in x direction= length(nm)/Mx

 y =y0+[0:My].'*dy;      % position of sample points in y direction

 h=1.0545715968;         % Planck's constant ( x 10^-34 unit in Js)
 hbar2=h^2;

 echarge=1.6021764628;   % electron charge ( x 10^-19 C)

baremass=9.10938188;     % bare electron mass (x 10^31 kg)

me1=m1*baremass;         % effective mass of carrier in GaAs
me2=m2*baremass;         % effective mass of carrier in InAs
const=hbar2/echarge;
```

```
deltax=xf/Mx;                % x-increment = length(nm)/n
deltax2=deltax^2;
const=const/deltax2;
mass=me1*ones(Mx+1,My+1);    % define the GaAs effective mass region
for i = 1:My-1;              % define the GaAs barrier region
    for j = 1:Mx-1;
        V(i,j)    =0.31 ;
    end
end

sizex=Mx/2;                  % define the midpoint of mesh

 for i = 25:My-25;           % define first InAs QD region
        for j = (sizex-n-10):(sizex-n)

         V(i,j)    =0;
        mass(i,j)  =me2;

         end
 end

 for i = 25:My-25;              % define second InAs QD region
     for j = (sizex+n):(sizex+n+10);
        V(i,j)    =0;
        mass(i,j)  =me2;
     end

end

V1=0.31*ones(Mx+1,My+1);
V1(2:Mx,2:end-1)=V(1:end,1:end);

return
```

BiQD_eigenergy.m

```
function[phi,te,d,num_sol,V1,V]=BiQD_eigenergy(d,num_sol,Mx,My,Vp,m1,m2);

% Call the function to define the region of QDs


[mass,V1,V,const]=call_BiQD(d,Vp,m1,m2,Mx,My);

 for  i=2:Mx-1;

          for  j=2:My-1;

d(i,j)=(((1/(mass(i1,j)+mass(i,j))+1/(mass(i+1,j)+mass(i,j)))+
(1/(mass(i,j-1)+mass(i,j))+1/(mass(i,j+1)+mass(i,j))))*const+ V(i,j));

% diagonal matrix element

offd1(i,j)=[(1/(mass(i-1,j)+mass(i,j)))] *const;

% off-diagonal matrix element

offd3(i,j)=[(1/(mass(i,j-1)+mass(i,j)))] *const;


          end
  end
```

```
for i=1:Mx-1;

            for j=1:My-1;

          offd2(i,j)=[(1/(mass(i+1,j)+mass(i,j)))] *const;

          offd4(i,j)=[(1/(mass(i,j+1)+mass(i,j)))] *const;

            end
  end

offd2(end,:)=zeros(1,My-1);

offd4(:,end)=zeros(My-1,1);


for i=2:Mx-1;

         for j=1:1;

d(i,j)=(((1/(mass(i1,j)+mass(i,j)))+1/(mass(i+1,j)+mass(i,j))

+(1/(mass(i,j)+mass(i,j))+1/(mass(i,j+1)+mass(i,j))))*const+ V(i,j));


offd1(i,j)=[(1/(mass(i-1,j)+mass(i,j)))] *const;

         end

end


for  i=1:1;

    for j=2:Mx-1;

d(i,j)  =-(((1/(mass(i,j)+mass(i,j))+1/(mass(i+1,j)+mass(i,j))

+(1/(mass(i,j-1)+mass(i,j)))+1/(mass(i,j+1)+mass(i,j))))*const+

V(i,j));

% diagonal matrix element

       offd3(i,j)=[(1/(mass(i,j-1)+mass(i,j)))] *const;

    end
end
      d(1,1)   = -(((1/(mass(1,1)+mass(1,1)))+1/(mass(2,1)+mass(1,1))+

(1/(mass(1,1)+mass(1,1))+1/(mass(1,2)+mass(1,1))))*const+ V(i,j));


          H=-(d(:))'; % diagonal matrix element
   offd1=(offd1(:))';  % off-diagonal element  1

   offd2=(offd2(:))';  % off-diagonal element  2

   offd3=(offd3(:))'   % off-diagonal element  3;

   offd4=(offd4(:))';  % off-diagonal element  4;

   Mx1=((Mx-1)*(My-1));


       for i=1:Mx1
         d(i)=H(i);
         offd1(i)=offd1(i);
         offd2(i)=offd2(i);
         offd3(i)=offd3(i);
         offd4(i)=offd4(i);
       end
```

```
        t = d(1:Mx1);
        t1 = -offd1(2:Mx1);
        t2 = -offd2(1:Mx1-1);
        t3 = -offd3(Mx:Mx1);
        t4 = -offd4(1:Mx1-(Mx-1));

  Hmatrix2=sparse(diag(t,0)+diag(t1,-1)+diag(t2,1)+diag(t3,-(Mx-1))+diag(t3,(Mx-1)));
  % Hamiltonian matrix

  [phi,te]=eigs(Hmatrix2,num_sol,'SM');      % Use Matlab function "eigs" to find
                                             % "num_sol" eigenfunctions and eigenvalues

  for i=1:size(phi,1)
      if (phi(i)<0)
    phi(i)=(-1)*phi(i);
       elseif (phi(i)>=0)
    phi(i)=(1)*phi(i);
       end
  end

 A= max(max(phi)); % Finding the maximum value of the wavefunction

 phi = phi./A;      % Finding the normalized amplitude of the wavefunction

  A= reshape(phi,Mx-1,My-1);
  Phi=zeros(Mx+1,My+1);
  Phi(2:Mx,2:end-1)=A(1:end,1:end);

return
```

Appendix B: List of Publications

International Journal

1. **N. Chit Swe**, O. Tangmattajittakul, S. Suraprapapich, P. Changmoang, S. Thanoi, C. Wissawinthanon, S. Kanjanachuchai, S. Ratanathammaphan and S. Panyakeow, "Improved quantum confinement of self-assembled high-density quantum-dot molecules in AlGaAs/GaAs quantum well structures by molecular beam epitaxy", *Journal of Vacuum Science and Technology B*, May 2008.

International Conference

2. **Nan Thidar Chit Swe**, Suwaree Suraprapapich, Chanin Wissawinthanon and Somsak Panyakeow, "Effect of the electric field on the linear polarization property of binary quantum dots", *Proceedings of the 2nd IEEE International Conference on Nano/Micro Engineered and Molecular Systems*, pp.1137-1140, January 2007.

National Conference

3. **Nan Thidar Chit Swe**, Suwaree Suraprapapich, Suphachok Thainoi, Pornchai Changmoang, Chanin Wissawinthanon and Somsak Panyakeow, "Polarized photoluminescence of InAs/GaAs linearly aligned quantum dots", *Thailand's 28th National Electrical Engineering Conference*, Vol.II, pp.1133-1136, October 2005.

4. **Nan Thidar Chit** Swe, Suwaree Suraprapapich, Chanin Wissawinthanon and Somsak Panyakeow, "Theoretical investigation on the optical polarization anisotropy of the photoluminescence from InAs/GaAs linearly aligned quantum dots", *Thailand's 29th National Electrical Engineering Conference*, Vol.II, pp.733-736, November 2006.

5. **Nan Thidar Chit Swe**, Suwaree Suraprapapich, Chanin Wissawinthanon, Somsak Panyakeow, and Charles Tu, "Excitation-Power and Temperature-Dependent Optical Properties of Binary Quantum Dots", *Thailand's 30th National Electrical Engineering Conference*, Vol. II, pp.953-956, October 2007. **(Best Paper Award)**

Vitae

Miss Nan Thidar Chit Swe was born in Yangon, Myanmar, on September 12, 1975. She received her B.Sc. (Honors) degree in Physics from Yangon University in 2000 and the M.Sc. degree in Engineering Physics from the same university in 2002, after which she became a faculty member there for two years before being granted a scholarship from the Japan International Cooperation Agency (JICA) for ASEAN University Network / South-East Asia Engineering Education Development Network (AUN/SEED-Net) in October 2004 for a Ph.D Sandwich Program in electrical engineering. She entered the Graduate School of Chulalongkorn University in November 2004 as a student of the Semiconductor Device Research Laboratory (SDRL), Department of Electrical Engineering, Faculty of Engineering. During January 2007 and September 2007, she got an opportunity to work as a visiting research student at the Research Center for Advanced Science and Technology, University of Tokyo, Japan, as part of the Ph.D. Sandwich Program. After completion of her Ph.D. degree, she is obliged to go back and work as a faculty member at Yangon University. Her research interest is in nanophotonics of III-V compound semiconductors.