Semiconductor Device Modeling and Simulation

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Lecture - 48
Problem Session-7

Hello, welcome to lecture number 48.

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So today we will take up some problem based whatever we have discussed in last week. Problem number 1. Show that for a degenerate semiconductor, relation between diffusion coefficient D and mobility mu is given by this expression. So in general if you write that current density is equal to q n times mu E, so that is a diffusion current density.

Similarly, for drift we can write J drift, so this is the drift current density, this is the diffusion. So diffusion current density will be related to the derivative of the carrier concentration. So it will be q times D times dn by dx for one dimension dn by dr for 3 where E is the electric field dn by dx is the derivative. Now if you compare these two, in equilibrium these both currents are equal if you consider the p n junction here, right?

So when it is in equilibrium the drift current and diffusion current are equal. So if you equate them what you will get, q n mu n times electric field is equal to q times d times

dn by dx or let us say this is subscript dn mu n be used because we are considering electrons here. Now instead of writing this electric field, we can use - q times E, which is the force on electron, which is the more general.

So we can write n times mu n minus times force on electron is equal to q times dn times dn by dx. So this is the equation. Let us take get away with the sign because we are comparing the main tours only. So if you take the ratio dn by mu n, it will be q times dn by dx divided by n times force. Now this force is related to the energy.

So the force in a semiconductor is can be written as minus del E F by del x where E F is minus q psi. So d psi by dx is the electric field minus d psi by dx. So this force will be related to the derivative of the energy. And we can substitute here. So this is q times dn by dx divided by n times del E F by del x. So now we can write dn by mu n is equal to q by n. Now both are dx dx cancel out.

So you have dn by d E F. Now if you recall if you take this derivative, so n is written as n i exponential E F minus E I by k T. So we take the derivative dn by E F what you will get? n i exponential E F minus E I by k T times 1 over k T. So this is basically n by K T. When we substitute here what you will get? This you will get q by n times n by K T. So this is the other way round, this is the inverse.

So this is q by K T. Now when we use this expression, this is valid for non-degenerate semiconductor. So the general expression is this and this which can also be written as n d E F by dn divided by q dn by dx. So this is basically n by q d E F by dn. Now this can also be written as n by if you take n out then we can write d E F by d of log n. Because d of log n is 1 over n dn.

So 1 over n dn can be written d of log n. So this is the expression for, a general expression. It is applicable for both, degenerate plus non-degenerate. And for non-degenerate we can use n equal to n i exponential E F minus E I by K T and then that simplifies to K T by q. So this is understanding that should be there.

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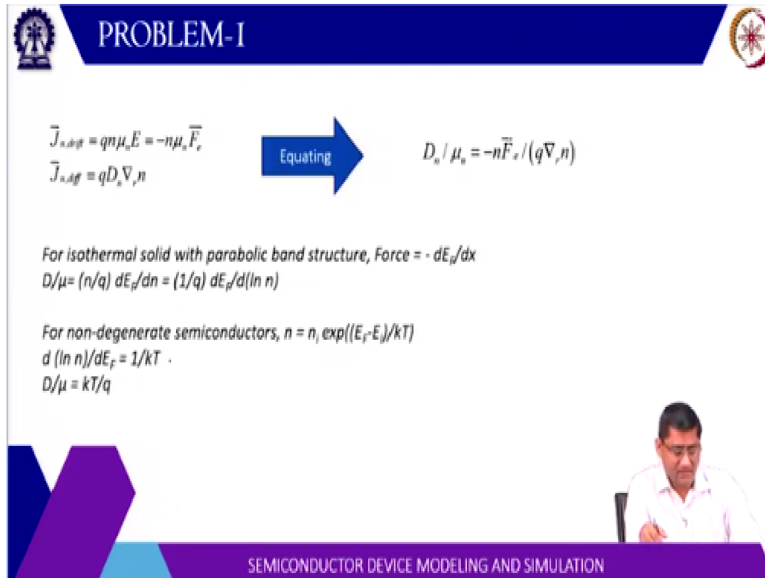

So this I have written here.

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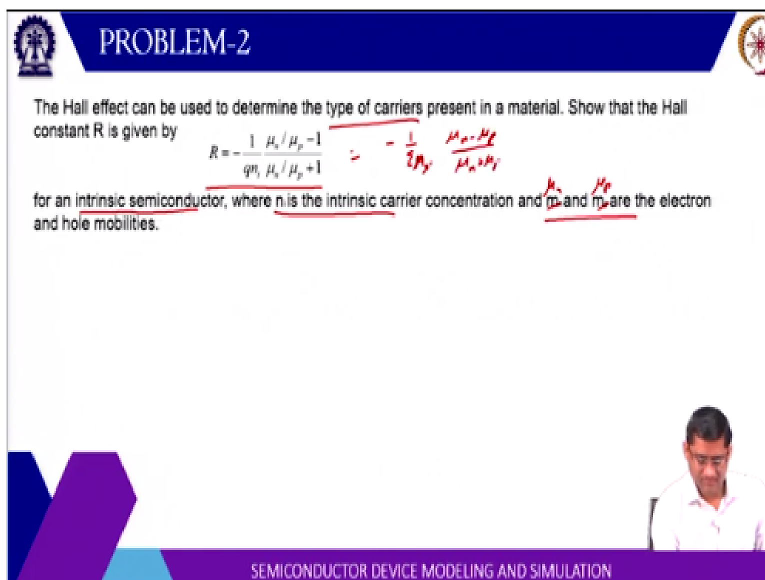

In the second one problem is the Hall effect can be used to determine the type of carriers present in the material. So Hall effect can be used to determine the type of carriers present in a material. Now so that Hall constants R is given by this equation. So Hall constant R can we measured from the other major quantities. So this is the expression for intrinsic semiconductor where n i is the intrinsic carrier concentration. m n, n p are the electron and hole.

And mu n and mu p are the electron and hole mobilities. So first let us understand what is the Hall effect.

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PROBLEM-2: Recall Hall Effect

(p-type material)

- $F = q(\mathcal{E} + v \times \mathcal{B})$ (Lorentz force)
- Net force in y-axis: $F_y = q(\mathcal{E}_y - v_x \mathcal{B}_z)$
- 0 current in y-direction
- $\rightarrow \mathcal{E}_y = v_x \mathcal{B}_z$
- $\mathcal{E}_y = (J_x/qp_0)\,\mathcal{B}_z = R_H J_x \mathcal{B}_z$
- Hall voltage
- $V_{AB} = \mathcal{E}_y w$
- Hall coefficient
- $R_H = \mathcal{E}_y/J_x\mathcal{B}_z = 1/qp_0$
- $V_{AB} < 0$ for n-type
- R_H and ρ yield majority carrier concentration and mobility

$$p_0 = \frac{1}{qR_H} = \frac{J_x\mathcal{B}_z}{q\mathcal{E}_y} = \frac{(I_x/wt)\mathcal{B}_z}{q(V_{AB}/w)} = \frac{I_x\mathcal{B}_z}{qtV_{AB}}$$

$$\rho(\Omega - \text{cm}) = \frac{Rwt}{L} = \frac{V_{CD}/I_x}{L/wt}$$

$$\mu_p = \frac{\sigma}{qp_0} = \frac{1/\rho}{q(1/qR_H)} = \frac{R_H}{\rho}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So consider a piece of semiconductor, a bar of semiconductor, where along the, this is the x axis, this is the y axis, this is the z axis. Along the x axis some potential is applied, let us say V applied and then current is flowing I x and the area of cross section we know this is w this is t and the length is some l. And there is a magnetic field in the z direction.

So due to this applied electric field current will flow and due to those magnetic field these carriers which are moving in this direction along the x axis will experience a Lorentz force. So that is v cross B. So if it is positive charge moving in this direction, so v cross B will be in this direction. And if it is negative charge moving in this direction, then the force will be in this direction because m a is equal to q into v cross B.

So v cross B in this direction and then this is negative here. So m a, so these charges will actually move in this direction. So net force on particle is q times electric field plus q times v cross v okay? Now in y direction there is no circuit here, there is nothing connecting here. So what will happen? This charge will just accumulate at the two boundaries creating a field which will oppose the Lorentz force.

So that means, the net force has to be zero. So F in y direction because there is no current flow, so F y has to be zero. That will be q times E in y direction minus q times v cross B. Now B we know is in z direction. So if v is in x direction so v cross v will

be in minus y direction. So this is the v cross v in minus y direction. So total force is this thing and they have to be equal. So you can also write E y is equal to v x v z.

So E y is equal to v x times v z. Now v x we can determine from the current because we know that j is equal to q n mu E. So mu is our drift velocity. So drift velocity is J by q n. So J by q p. Now p if this is a hole, holes of the carrier then J by q p. So you can use this expression. So here we are using p type material. So we can use J by q p. Now E y is J by q p times B z.

Now B z is applied we know. E y we know because we have reapplied an L. So E will be, E y will be V applied by L. Then J x we can measure. That will be I x times per unit area. So area will be w times t. So I x we can measure, J x we can calculate. E y also we can calculate and B z is the applied magnetic field that also we know. So the ratio of E y by J x B z, we can find out.

And that will be equal to 1 by q p naught. So by measuring these three quantities, applying the magnetic field B z, applying the V applied and then measuring the J x and E y we can calculate 1 by q p naught which is Hall coefficient. Now this is for p type material. What if both the carriers are there? Then what we will have to do? We will have to write the equation for both the carriers.

So this is a more general case. Okay, another thing you can notice here for p type carrier, V ab is positive basically. For p type this is for, because holes are moving in this direction and then v cross B is in this direction so the holes accumulate here. If there are electrons, then if current flows in x direction, then these electrons will move in minus x direction. So v cross B will be in this direction.

So they will accumulate to the this side, right? No, because v cross B is in y direction, but the force is q times v cross B and the charge on electrons is minus q. So y direction multiplied by minus q. So it will be again in minus y direction only. So whether there are holes carrier or there electron carriers, they both will be deflected in minus y direction due to this B z because this is q times v cross B.

So q and v so both are positive for holes and both are negative for electrons. So essentially both will be forced in this direction only. So that means, if you measure this voltage V ab so that is E y will be V ab this is E x. E y will be V ab divided by w. So this will be positive for p type and negative for n type. So that means this R H will also have again the same sign.

It will be positive for p type negative for n type. And this yields a majority carrier concentration and the mobility. So from these two measurements, the R H you can measure E y and J x. So by J x and E y you can find the carrier concentration. Then when you substitute this carrier concentration in J y equation, you can find out the mobility. So for one type material this can be found out. Now let us say both type of materials are there.

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PROBLEM-2: Recall Hall Effect

- Hall effect (general)
- $F_{hy}=eE_y-ev_{hx}B_z=ev_{hy}/\mu_h$
- $-F_{ey}=eE_y+ev_{ex}B_z=ev_{ey}/\mu_e$
- $J_y=epv_{hy}+env_{ey}=0$
- $J_x=epv_{hx}+env_{ex}$
- $R_H=E_y/J_xB_z$

$$R_H = \frac{p\mu_h^2 - n\mu_e^2}{e(p\mu_h + n\mu_e)^2}$$

- accurate expression including Hall scattering factor r_e and r_h using ($J_y=r_e epv_{hy}+r_h env_{ey}=0$),

$$R_H = \frac{r_h p - r_e b^2 n}{e(p + bn)^2},$$

DEVICE MODELING AND SIMULATION

So now here if you see here, again the same scenario basically. The voltage is applied and in the x direction current is flowing and the magnetic field is in B z direction and both electron and holes they will experience force in - y direction due to q into v cross B. And then there is a value in net resultant electric field and this electric field will be in the opposite direction for the electrons and holes.

So what we write? We write this force equation in y direction for both electrons and holes and that will be electric field minus the force due to magnetic field. So E e minus q into v cross B. And that can be written as if you recall v is equal to mu times

e okay or it can be written as mu times force by e where e is the force. So now this force is more general term. So that is E e plus E times v cross B.

So this is v is equal to ev hy mu h. So this is written here basically, ev by mu this force is written as ev by mu. So we can write this equation for both electrons as well as holes in y direction. Then for x direction J x is epv hx env ex. So this electron drift velocity in x direction then their concentration plus hole drift velocity in the x direction and their concentration.

So this is the current density in x direction. This is the current density in y direction. But in y direction there is no circuit. So the current density has to be zero. So epv hy plus env ey equal to zero. And from these two equations of the force we can enter the value of v hy vy to this expression. And then of course, when we evaluate R H equal to E y by J x B z, this is same formula.

And so there are 1 equation 2 equation and this let us say these are 3 and 4 equation. So 3 and 4 are substituted to 2. And when we evaluate this one, we get p times mu h square minus n times mu e square divided by e times p mu h plus n mu e whole square. So this is the expression for all coefficient. Now if you consider a intrinsic semiconductor, intrinsic semiconductor.

So in intrinsic p is equal to n equal to n i. So if you substitute this in here. So what you have here, n i times mu h square minus mu e square divided by e times n i square times mu h plus mu e whole square. So this can be simplified as n i, 1 and i will cancel. So you will have e times n i in the denominator and mu h plus mu e and in numerator mu h minus mu e. So this is the same expression that was asked, okay?

1 by q n i times mu h by mu; mu h minus mu p this can be written as minus 1 over q n i plus mu n minus mu p divided by mu n plus mu p. So this is same expression, mu x minus mu by e n i mu h plus mu p. So this can be derived. Now some advanced effect they consider the Hall scattering. So Hall scattering is arising because there is a magnetic field applied here.

So there is a different scattering probabilities there, because if you recall in previous problem we discussed that J is some kind of sigma times E, right? And then we have sigma xx sigma xy. So sigma xx was due to electric field. Sigma xy was due to magnetic field. And it has a term some tau square, okay. So the hole is scattering is slightly different. So instead of writing this expression equation 2 we multiply this thing by some scattering coefficient.

So J y is written r e times epv hy plus r h times ep ey where r e and r h has the electron and hole scattering factor. And then again using this expression if you evaluate, you get these factors here. So r h p minus r e. N b is mu here b is mu e by mu h. So the same expression. The only thing is that mu is multiplied by with r e and mu h is multiplied by um R H. So this expression you will get.

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Now what is the significance of this scattering factor, electron and hole scattering factor? They are basically the ratio of mu h by mu c. So this is the hall mobility and this is the conduction mobility. So conduction mobility expression we use in conduction current. So J is equal to n e mu e. So they are the mu e is conduction mobility.

And in case of Hall effect we are using some mobility expression here v is equal to mu E so that is Hall mobility. So v hy will be mu h times e y. And v hx will be mu conduction times e x. So if you check the ratio now we know that mu is equal to q

average tau by m. But in case of this is mu conduction. In case of mu h, we had actually tau square. So it is basically related to tau square, average of tau square.

So what we do? Here we take the average of tau square and here is basically tau average whole square. So this is the difference. Now this comes because the scattering mechanism is coming into the picture here. And if you check the scattering mechanism so for parabolic band structure or with spherical constant energy surfaces, tau m is e to the power minus r for phonon scattering.

And it is e to the power minus 3 by 2 for ionized impurity scattering. So tau to the power n, average of tau to the power n will be tau to the power n e to the power 3 by 2 exponential minus E by k T. So this expression if you evaluate, so if you use substituted here, then Hall scattering factor will be 1.18 for phonon and around 1.93 for ionized impurity scattering.

And there is a magnetoresistance effect also. That means under a strong magnetic field there is significant increase in the resistivity. Now why it is happening? Because let us say you apply electric field and then v is equal to mu e. So this electron is supposed to move in a straight line. But let us say you have some magnetic field. Now these electrons will not take a straight path, because this magnetic field will you know apply a perpendicular field force.

So they will you know take a longer path basically, because this magnetic force is basically forcing them away from this path or in the direction of the field. So due to this longer path, the resistance actually increases and this is called magnetoresistance effect, okay?

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PROBLEM-4

Solve poisson equation 2D : $-\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)=20\cos(3\pi x)\times\sin(2\pi y)$ for $x=[0,1]; y=[0,1]$

Dirichlet boundary (lext and right edge)

$u(x=0)=0$

$u(x=1)=0$

Neumann boundary for y-axis (upper and lower edge) $\frac{\partial u}{\partial n}=0$

```
%--Define the 2D mesh
loop=1;
N=20; Nx=N; Ny=N;
xa=0; xb=1; ya=0; yb=1;
dx=(xb-xa)/(Nx-1);
dy=(yb-ya)/(Ny-1);
%% since dx = dy we can use h = dx = dy
h=dx;
M=400; % maximum iteration value
```

```
%--Initialize
V(1:Nx,1:Ny)=0.0;
f(1:Nx,1:Ny)=0.0;
for i=1:Nx,
for j=1:Ny,
f(i,j)=20*cos(3*pi*(xa+(i-1)*dx))*sin(2*pi*(ya+(j-1)*dy));
end
End
% Boundary conditions
V(1,:)=0;
V(Nx,:)=1; %% Dirichlet in x
g=0; %% Neumann in y
```

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So we have discussed three problems. Now fourth problem is related to solving the some differential equation. Here we are solving some kind of Poisson equation okay. It is not from the semiconductor, but we have defined some simpler forcing function. So it is a d2 psi by dx square where psi is written as u basically. So d2 u by dx square plus d 2 u by d y square is a 2d.

So it is a 2d is equal to 20 cosine 3 pi x plus sine 2 pi x. So this is your forcing function. Then the domain is x equal to 0 to 1 and y equal to 0 to 1. So this is your domain here. So this is x 0 to 1. This is y 0 to 1. Now there are boundary conditions here. At x equal to 0 there is a Drichlet boundary condition. So this is 0 here. At x = 1 this point here this is also Drichlet boundary condition, this is 0 here.

And in y direction du by dn, so this is basically du by dy okay because this will be dy, is equal to 0 for upper and lower edges. So we have two Drichlet boundaries and two Neumann boundaries. So the how do we proceed? So first we define the mesh. So we define the mesh. So let us choose number of points. Let us say there are 20 grid points in x direction, there are 20 grid points in y direction.

So you can just change this number to have more or less grid. When you develop a code you start with some n equal to 4 or 5 so that you can actually see you know what is happening, you can debug it. But then later on you increase the number to get a better solution, but start with a small number. Then xa is 0, xb is 1, ya is 0, yb is 1. So this is xa, this is xb, this is ya, this is yb.

Then dx is this gap divided by n minus 1 because if you see here, let us say n equal to 2, then you will not have any middle point. So these are the two points and the dx is basically a minus b by 1. So this is basically a minus b by n minus 1. So for both x and y. Then of course, here we use, we have used uniform grid. So dx equal to dy, let us call it H. So H is equal to dx.

Now M is the number of iteration. We are going to solve it iteratively, okay and we are expecting that within you know few hundred iteration it will converge. So let us set it to 400 because if you do not set this number and if you just satisfy the just specify the criteria that you know it will converge, then we will stop, it will not converge. So then it will go on you know then you have to terminate forcefully and which is not good.

So we specify some number of iterations that after which we expect it to converge. Then we initialize. So we initialize that v is 0. So v is basically the u, v is basically this u here. So v is 0. Then f is 0, this is f here. So we initialize. Then what we do? Then we specify the f. So for i equal to 1 to n x j equal to 1 to n by f i j is 20 cos 3 pi x and x is xa plus i minus 1 dx. And y is ya plus j – 1 dy.

So that way we have specified this f function. So for all the grid points, we have to find out v and we have to find out f. f we have already found out because this is straightforward. It is a function of position only. So from this code, we have initialized v to be 0 and f we have calculated from the right hand side. Then now we apply the boundary condition. So boundary condition means, this column has to be 0.

So v 1 comma column. So this is your v basically. And if you see here, these are the grid points. So this column correspond to x equal to 0. So x equal to 0 this is 0 and v at x N x column is 1. Actually this boundary condition is 1 here, it is not 0 because in the code it is specified as 1. So N x column and first column. So first column is 0, N x column is 1. So this boundary condition is 1 here.

That is Drichlet in x direction. Then in y direction this we call g. So g is 0 here, derivative. G is 0 here. So that has to include in the discretization because, if you

recall that discussion on Neumann boundary, we modified the differential equation in such a way that this g was included.

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PROBLEM-4

```
w=cos(pi/Nx)+cos(pi/Ny); % Converging Term
Ncount=0;
loop=1;
while loop==1;
 Rmin=0;
j=1;
for i=2:Nx-1
 Residue=w.*(0.25.*(V(i-1,j)+V(i+1,j)+2*V(i,j+1)+2*g*h+(h^2)*f(i,j))-V(i,j));
 Rmin=Rmin+abs(Residue);
 V(i,j)=V(i,j)+Residue;
end
for j=2:Ny-1
for i=2:Nx-1
 Residue=w.*(0.25.*(V(i-1,j)+V(i+1,j)+V(i,j-1)+V(i,j+1)+(h^2)*f(i,j))-V(i,j));
 Rmin=Rmin+abs(Residue);
 V(i,j)=V(i,j)+Residue;
end
end
j=Ny;
for i=2:Nx-1
 Residue=w.*(0.25.*(V(i-1,j)+V(i+1,j)+2*V(i,j-1)+2*g*h+(h^2)*f(i,j))-V(i,j));
 Rmin=Rmin+abs(Residue);
 V(i,j)=V(i,j)+Residue;
end
Rmin=Rmin/(Nx*Ny); % Average Residue per grid point
if(Rmin>=0.00001)
 Ncount=Ncount+1;
 if(Ncount>M)
  loop=0;
  disp(['solution doesnt converge in ',num2str(M),' iter'])
 end
else
 loop=0;
 disp(['solution converges in ',num2str(Ncount),' iteration'])
end
end
```

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So and then if you recall the discussion on successive over relaxation Newton method omega was some parameter for relaxation. So here omega is defined as cos pi by Nx plus cos pi by Ny. This is one criteria. So here we have used it. Then we start the counting. So let us say N count is 0 and this is the first loop. Now while the loop is 1 and R minimum is 0. So while the loop is 1 we against set R minimum equal to 0.

And for first row, so your v is in this. So first column and last column we have already made 0. Now for first row, here we will have point outside this one. So we will have 2gh there right? So you recall this was 4 v i, j minus the near neighbors v (i – 1, j) – v (i + 1, j) – v(i, j – 1) - v (i, j + 1). So this is i, this is j. So j – 1 will be outside this one okay? So this was replaced by v(i, j + 1) + 2gh.

So you will have two times i, j + 1. So you see here this is v (i, j) + v(i + 1, j) + 2v i, j+ 1 + 2gh. Then plus h square times f is equal to v ij because this was equal to h square f i, j So this expression is written for the first one. So what we have done instead of taking this 4 we divide whole thing by 4. So v ij coefficient become 1 and rest are divided by 4. So then, if you recall we wrote that w is equal to m times w, that format right?

So it is basically we are having this residue here. So v ij minus the estimate of v ij. So that is the residue, the difference. So v ij is equal to something, some term the collection of all these term. So if you rearrange here, so v ij is written as 1 by 4 times h square f plus v i minus 1, j plus v i plus 1, j plus 2v i, j plus one plus 2 gh. So this is the estimate of v ij.

So when we subtract we get delta v ij. So this is basically delta v ij multiplied by the residue w by this the relaxation parameter w. So then your residue R min is updated, R min is added with absolute value of this residue. So this is the residue for first row. Then we update the voltage v ij plus residue. So your v ij this is the next estimate of v ij. Then for the second to second last row, these are the internal points.

So for internal points we do not have any boundaries. So we can straightaway use this equation without 2 gh. So all the neighbors i – 1, i + 1, j – 1, j + 1 plus h square fj and this is the residue. And we again update these individual points with a residue and this overall residue we are adding it basically with residue. And then for the last row again same thing.

Here will be j – 1 and then 2 gh for the last row because there will be fixed point here at j + 1. So j + 1 is replaced by j - 1 and 2 + 2 gh. And then again the residue is added and v ij are updated. Then what we do? We divide this residue by the number of points N x, N y to get the average residue per grid.

And then this is some parameter that if the residue is less than some 10 raised to power minus 1, 2, 3, 4, 5; 10 raised to power -5 be converged. We say it is converged. So if it is greater than this, then we will again. So n count is increased, n count plus 1. And if n count is more than m then of course, we stop because it has not converged.

And otherwise, if R minimum is less than this number, then we close this one. Solution converges in this many iterations and we display the solution.

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PROBLEM-4

```
% Plot the result
X=xa:dx:xb;%1:Nx;
Y=ya:dy:yb; %1:Ny;
mesh(X,Y,V','linewidth',2)
h=gca;
get(h,'FontSize');
set(h,'FontSize',16);
%colorbar('location','eastoutside','fontsize',12);
%axis([1 Nx 1 Ny])
xlabel('X','fontSize',16);
ylabel('Y','fontSize',16);
title('Electric Potential Distribution, V(X,Y)','fontsize',20);
fh = figure(1);
set(fh, 'color', 'white');
```

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

How do we display the solution? So now we plot it. Now we define these vectors X is equal to xa to xb in the step of dx; y is equal to ya to yb in the steps of dy. Then we generate a 2d mesh with xy and plot v in it. So let us say h is this is basically for some kind of handle. Then we plot it, here this mesh will actually plot, this v is plotted on x pi grid. So if you see here, this is x = 0, this is x = 1.

The values are 0 here, this is your v. Values are 1 here. And then if you see this boundary y = 0, this is y = 0 and this is y = 1. So this is see this derivative is 0 here as we specified in the solution. So this is flat basically. And then you get this variation. This variation is coming due to the nature of the forcing function. Forcing function is what? Cos 3 pi x and sine 2 pi y.

So if you plot cos 3 pi x and sine 2 pi y. So cos 3 pi x 0 to 1. So 0 to 1, this is 1. So it will be cos 3 pi. So it will take you know some number of terms here. So if you see here there is a maxima, there is a minima, there is a maxima again right? So it is some kind maxima, minima and maxima, right? So this is something like 3 pi by 2.

And then if you see sine 2 pi y, so this is y this is x. Sine 2 pi y, now cos is 1 here actually. So it will start with some kind of maxima here. But it should start with maxima here, but because of this boundary condition it is 0 actually. Now it is multiplied by sine 2 pi y, so sine will start with 0 and at y equal to 0 it will be 0. And then 2 pi y means 0 to 2 pi. So 0 to pi and 0 to 2 pi.

So this is how sine variation in y will basically go, okay? So you see here, this variation you can see here, okay? Here is multiplication of sine and cosine. So that is why this is reverse basically. So that variation you can see the effect of the forcing function. So in this lecture, we have discussed four problems. One is related to the d by mu, other is related to the Hall effect.

And of course, one with the solution of this Poisson equation, how to solve the Poisson equation for a xy in 2d space xy grid. So thank you very much.