ECE606: Solid State Devices
Lecture 13
Solutions of the Continuity Eqs. Analytical & Numerical

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Outline

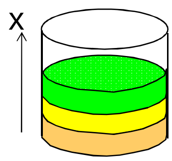
Analytical Solutions to the Continuity Equations

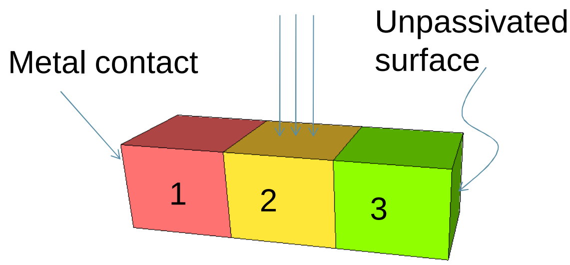
1) Example problems
2) Summary

Numerical Solutions to the Continuity Equations

1) Basic Transport Equations
2) Gridding and finite differences
3) Discretizing equations and boundary conditions
4) Conclusion

Consider a complicated real device example





- Acceptor doped
- Light turned on in the middle section.
- The right region is full of mid-gap traps because of dangling bonds due to un-passivated surface.
- Interface traps at the end of the right region (That's where the dangling bonds are…)
- The left region is trap free.
- The left/right regions contacted by metal electrode.

Recall: Analytical Solution of Schrodinger Equation

1) $$\frac{d^2\psi}{dx^2}+k^2\psi=0$$ → 2N unknowns for N regions

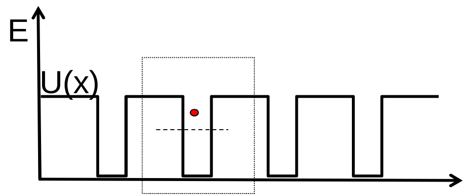
2) $$\psi(x=-\infty)=0 \qquad \psi(x=+\infty)=0$$ → Reduces 2 unknowns

3) $$\psi\big|_{x=x_B^-}=\psi\big|_{x=x_B^+} \qquad \left.\frac{d\psi}{dx}\right|_{x=x_B^-}=\left.\frac{d\psi}{dx}\right|_{x=x_B^+}$$ → Set 2N-2 equations for 2N-2 unknowns (for continuous U)

4) Det(coefficient matix)=0 And find E by graphical or numerical solution

5) $$\int_{-\infty}^{\infty}\left|\psi(x,E)\right|^2 dx=1$$ for wave function

Recall: Bound-levels in Finite well

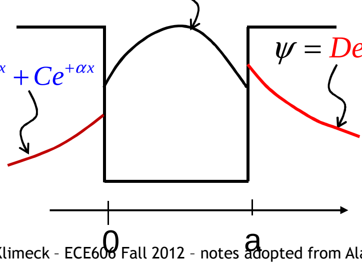


1)

$$\psi = A\sin kx + B\cos kx$$

$$\psi = \cancel{Me^{-\alpha x}} + Ce^{+\alpha x}$$

$$\psi = De^{-\alpha x} + \cancel{Ne^{+\alpha x}}$$



2) Boundary Conditions

$$\psi(x = -\infty) = 0$$

$$\psi(x = +\infty) = 0$$

Analogously, we solve for our device

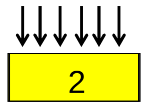
Solve the equations in different regions independently.

Bring them together by applying boundary conditions.

Region 2: Transient, Uniform Illumination, Uniform doping

$$\frac{\partial n}{\partial t}=\frac{1}{q}\cancel{\nabla\bullet\mathbf{J}_N}-r_N+g_N \qquad \mathbf{J}_N=qn\mu_N E+qD_N\nabla n$$

(uniform)



Acceptor doped

$$\frac{\partial(\cancel{n_0}+\Delta n)}{\partial t}=-\frac{\Delta n}{\tau_n}+G$$

Recall Shockley-Read-Hall

$$\frac{\partial p}{\partial t}=\frac{-1}{q}\cancel{\nabla\bullet\mathbf{J}_p}-r_P+g_p \qquad \mathbf{J}_p=qp\mu_p E-qD_P\nabla p$$

(uniform)

$$\frac{\partial(\cancel{p_0}+\Delta p)}{\partial t}=-\frac{\Delta p}{\tau_p}+G$$

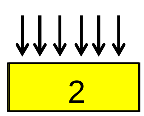
Majority carrier

Electric field still zero because new carriers balance

$$\nabla\bullet D=q\left(p-n+N_D^+-N_A^-\right)=q\left(p_0+\Delta n-n_0-\Delta p+N_D^+-N_A^-\right)=0$$

Example: Transient, Uniform Illumination, Uniform doping, No applied electric field

$$\frac{\partial(\Delta n)}{\partial t}=-\frac{\Delta n}{\tau_n}+G$$



Acceptor doped

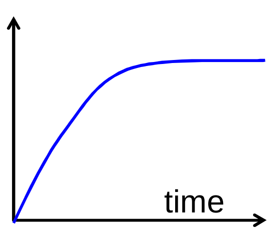
$$\Delta n(x,t)=A+Be^{-t/\tau_n}$$

No carriers yet generated…

$$t=0,\quad \Delta n(x,0)=0\Rightarrow A=-B$$

$$t\rightarrow\infty,\quad \Delta n(x,\infty)=G\tau_n=A$$

Steady state, no change in carriers with time…



$$\Delta n(x,t)=G\tau_n\left(1-e^{-t/\tau_n}\right)$$

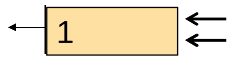
Region 1: One sided Minority Diffusion at steady state

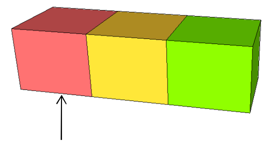
$$\frac{\partial n}{\partial t} = 0 (\text{steady-state})$$

$$r_N = 0 (\text{trap free})$$

$$g_N = 0 (\text{nogeneration})$$

Steady state
Acceptor doped





Trap-free

$$\cancel{\frac{\partial n}{\partial t}} = \frac{1}{q}\frac{dJ_n}{dx} - \cancel{r_N} + \cancel{g_N}$$

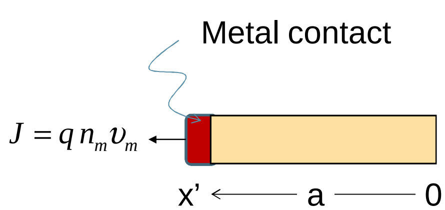
$$E = 0 \qquad \mathbf{J}_N = qn\cancel{\mu_N}E + qD_N\frac{dn}{dx}$$

$$\left.\begin{matrix} \\ \\ \end{matrix}\right\} \quad 0 = D_N\frac{d^2n}{dx^2}$$

$$D_N\frac{dn}{dx} \neq 0 \text{ (due to insertion of electrons from central region)}$$

Example: One sided Minority Diffusion

$$0 = D_N\frac{d^2n}{dx^2}$$



$$\Delta n(x,t) = C + Dx'$$

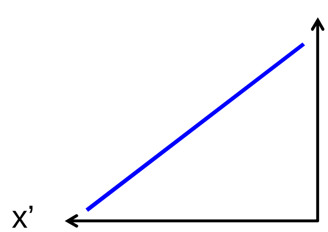
$$x = a, \quad \Delta n(x' = a) = 0 \Rightarrow C = -Da$$

(Metal has high electron density
as compared to semiconductor)

$$x = 0', \quad \Delta n(x' = 0') = C$$

Just substitute x=0 in above eqn.

$$\Delta n(x,t) = \Delta n(x = 0')\left(1 - \frac{x'}{a}\right)$$

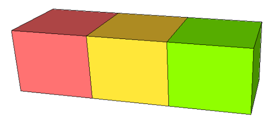


Region 3: Steady state Minority Diffusion with recombination

$$\frac{\partial n}{\partial t} = 0 (\text{steady-state})$$

$$r_N \neq 0 (\text{not trap free})$$

$$g_N = 0 (\text{nogeneration})$$

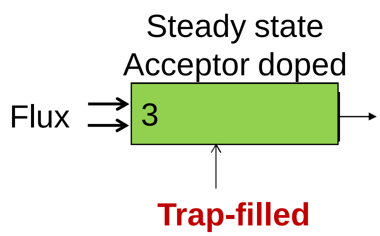


$$E = 0$$

$$D_N \frac{dn}{dx} \neq 0 \text{ (due to insertion of electrons from central region)}$$

$$0 = D_N \frac{d^2(n_0 + \Delta n)}{dx^2} - \frac{\Delta n}{\tau_n}$$

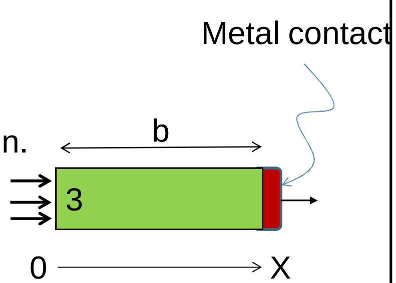
$$0 = D_N \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n}$$



Diffusion with Recombination ...

$$D_N \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} = 0$$

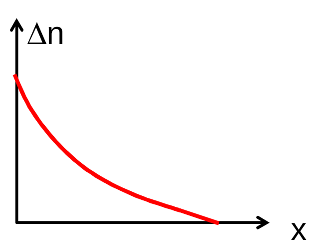
Functionally similar to Schrodinger eqn.



$$\Delta n(x,t) = E e^{x/L_n} + F e^{-x/L_n}$$

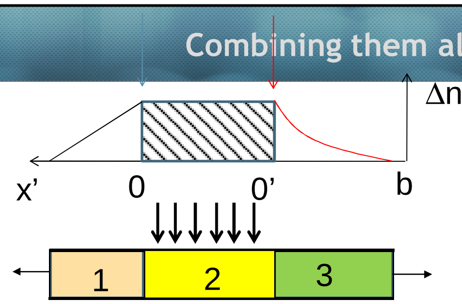
$$x = b, \quad \Delta n(x=b) = 0 \quad \Rightarrow F = -E e^{2b/L_n}$$

$$x = 0, \quad \Delta n(x=0) = E + F = \Delta n(x=0)$$



$$\Delta n(x,t) = \frac{\Delta n(0)}{(1 - e^{2b/L_n})} (e^{x/L_n} - e^{2b/L_n} e^{-x/L_n})$$

Combining them all ....



$$\Delta n_2(x) = G\tau_n =$$
$$\Delta n_2(0) = \Delta n_2(0')$$

Match boundary condition

$$\Delta n_1(x') = \Delta n(x=0)\left(1 - \frac{x'}{a}\right) = G\tau_n\left(1 - \frac{x'}{a}\right)$$

$$\Delta n(x) = \frac{\Delta n(0')}{(1 - e^{2b/L_n})}(e^{x/L_n} - e^{2b/L_n}e^{-x/L_n}) = \frac{G\tau_n(e^{x/L_n} - e^{2b/L_n}e^{-x/L_n})}{(1 - e^{2b/L_n})}$$

Calculating current $\quad \mathbf{J}_N = qn\mu_N E + qD_N \frac{dn}{dx}$

Analytical Solutions Summary

1) Continuity Equations form the basis of analysis of all the devices we will study in this course.

2) Full numerical solution of the equations are possible and many commercial software are available to do so.

3) Analytical solutions however provide a great deal of insight into the key physical mechanism involved in the operation of a device.

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1) Example problems
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Numerical Solutions to the Continuity Equations

1) Basic Transport Equations
2) Gridding and finite differences
3) Discretizing equations and boundary conditions
4) Conclusion

Preface

- The 5 equations we derived the past few lectures have been used for the longest time in the industry and in academia to understand carrier transport in devices.
- It is useful to know the essentials of how these equations are *implemented* on a modern computer so that one understands some of the finer details involved in creating tools that simulate thee phenomena.
- Understanding some of these details helps one become a 'power user' of the simulation tools that implement the physics. One also understands the limitations re. numerical issues and applicability ranges of results.

Equations to be solved - derived last time.

$$\nabla \bullet D = q\left(p - n + N_D^+ - N_A^-\right)$$ ← Band-diagram

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \bullet \mathbf{J}_N - r_N + g_N$$

$$\mathbf{J}_N = qn\mu_N E + qD_N \nabla n$$

$$\frac{\partial p}{\partial t} = \frac{-1}{q}\nabla \bullet \mathbf{J}_P - r_P + g_P$$

$$\mathbf{J}_P = qp\mu_P E - qD_P \nabla p$$

← Diffusion approximation, Minority carrier transport, Ambipolar transport

1) The Semiconductor Equations

Conservation Laws: not specific to a particular problem - Universal

$$\nabla \bullet \vec{D} = \rho$$

$$\nabla \bullet \left(\vec{J}_n / -q\right) = \left(g_N - r_N\right)$$

$$\nabla \bullet \left(\vec{J}_p / \ q\right) = \left(g_P - r_P\right)$$

(steady-state)

Constitutive relations: specific to problem at hand – reflect physics of the problem

$$\vec{D} = \kappa\varepsilon_0 \vec{E} = -\kappa\varepsilon_0 \vec{\nabla} V$$

$$\rho = q\left(p - n + N_D^+ - N_A^-\right)$$

$$\vec{J}_n = nq\mu_n \vec{E} + qD_n \vec{\nabla} n$$

$$\vec{J}_p = pq\mu_p \vec{E} - qD_p \vec{\nabla} p$$

$$g_{N,P} = f(n, p) \text{ etc.}$$

The "Semiconductor Equations"

$$\nabla \bullet \vec{D} = \rho$$

$$\nabla \bullet \left(\vec{J}_n / -q\right) = \left(g_N - r_N\right)$$

$$\nabla \bullet \left(\vec{J}_p / q\right) = \left(g_N - r_N\right)$$

3 coupled, nonlinear, second order PDE's for the 3 unknowns:

$V(\vec{r})$ $n(\vec{r})$ $p(\vec{r})$

Why are these equations coupled?
Potential→Field→current→changes potential→changes field and so on…

Conservations laws: **exact**
Transport eqs. (drift-diffusion): **approximate**

Analytical Solutions to the Continuity Equations

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Numerical Solutions to the Continuity Equations

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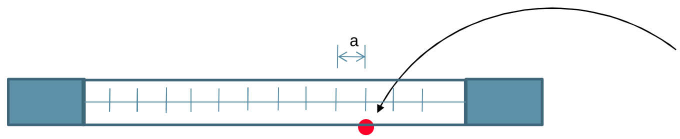
2) The Grid

(ii) "exact" numerical solutions

N nodes
3N unknowns



V_i

n_i

p_i

'Gridding'– total length divided into 'N' parts
- equal (uniform gridding) , or
- unequal (adaptive and non-uniform gridding)

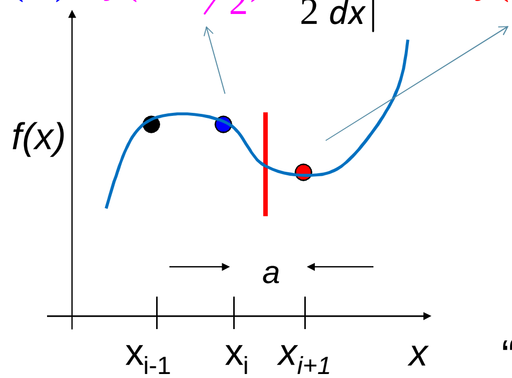
Variables described at each point '*i*'.

V_o and V_{n+1} is known because these are voltages at source and drain.

Finite Difference Expression for Derivative

$$f(x_o) = f(x_o + a/2) - \frac{a}{2}\frac{df}{dx}\bigg|$$

$$f(x_o + a) = f(x_0 + a/2) + \frac{a}{2}\frac{df}{dx}\bigg|$$



$$\frac{df}{dx}\bigg|_{(x_{i+1/2})} = \frac{f_{i+1} - f_i}{a}$$

"centered difference"

The Second Derivative ...

$$f(x_0+a) = f(x_0) + a\left.\frac{df}{dx}\right|_{x_0=a} + \frac{a^2}{2}\left.\frac{d^2f}{dx^2}\right|_{x_0=a} + \ldots$$

$$f(x_0-a) = f(x_0) - a\left.\frac{df}{dx}\right|_{x_0=a} + \frac{a^2}{2}\left.\frac{d^2f}{dx^2}\right|_{x_0=a} - \ldots$$

$$f(x_0+a) + f(x_0-a) - 2f(x_0) = a^2\left.\frac{d^2f}{dx^2}\right|_{x_0=a}$$

$$\left.\frac{d^2f}{dx^2}\right|_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{a^2} \longrightarrow$$

3 point formula, could be extended to N points depending on the number of derivatives we carry in our expansion

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Analytical Solutions to the Continuity Equations

1) Example problems
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Numerical Solutions to the Continuity Equations

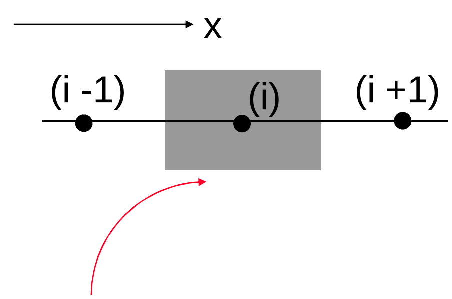
1) Basic Transport Equations
2) Gridding and finite differences
3) **Discretizing equations and boundary conditions**
4) Conclusion

2) Control Volume

3 unknowns at each node:

$$V_i, n_i, p_i$$

Need 3 equations at each node



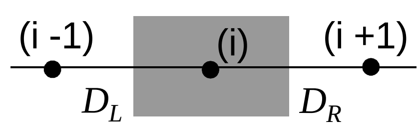
Discretizing Poisson's Equation

$$\nabla^2 V = -\rho / K_s \varepsilon_o$$

$$\nabla \bullet D = \rho \qquad D = K_s \varepsilon_0 \mathcal{E} = -K_s \varepsilon_0 \nabla V$$

$$\frac{V_{(i-1)} - 2V_{(i)} + V_{(i+1)}}{a^2} = -\frac{q}{K_s \varepsilon_0}\left(p_i - n_i + N_{D,i}^{+} - N_{A,i}^{-}\right)$$

Since V_0 and V_{-1} are known, as are carrier concentration on doping (or lack thereof) in contacts, we find V_1 and iterate from this point to solve for potential.

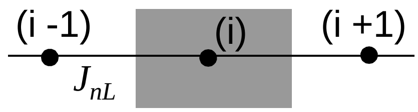


$$F_V^i\left(V_{i-1}, V_i, V_{i+1}, n_i, p_i\right) = 0$$

→ Once this potential is found, solve continuity equation to obtain new carrier concentrations

Discretizing Continuity Equations

$$\nabla \bullet \vec{J}_n = -q\left(g_N - r_N\right)$$



$$J_{nL} = -nq\mu_n \frac{dV}{dx} + kT\mu_n \frac{dn}{dx}$$

The simplest approach…..

$$\frac{J_{nL}}{kT\mu_n} = -\left(\frac{n_{i-1}+n_i}{2}\right)\left(\frac{V_i - V_{i-1}}{a\left(kT/q\right)}\right) + \left(\frac{n_i - n_{i-1}}{a}\right)$$

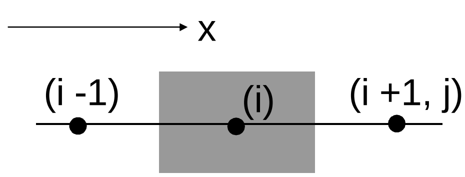
$$F_n^i\left(V_{i-1}, V_i, n_i, n_{i-1}, p_i, p_{i-1}\right) = 0$$

Three Discretized Equations

$$F_V^i = 0$$

$$F_n^i = 0$$

$$F_p^i = 0$$



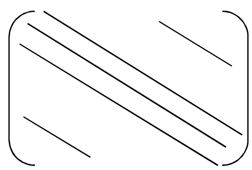
3 unknowns at each node
N nodes
3N unknowns and 3N equations (coupled to each other)

Numerical Solution - Poisson Equation Only

- Have a system of 3N nonlinear equations to solve
- Recall Poisson's equation at node (i):

$$F_V^i\left(V_{i-1}, V_i, V_{i+1}, n_i, p_i\right) = 0$$

<u>linear</u> if n_i and p_i are known $[A]\vec{V} = \vec{b}$

[A]: 

$$\vec{V} = \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_N \end{bmatrix}$$

Boundary conditions

Contacts are assumed large and in equilibrium → detailed balance and law of mass-action apply!!

$$n_0 p_0 = n_i^2 \qquad n_{N+1} p_{N+1} = n_i^2$$

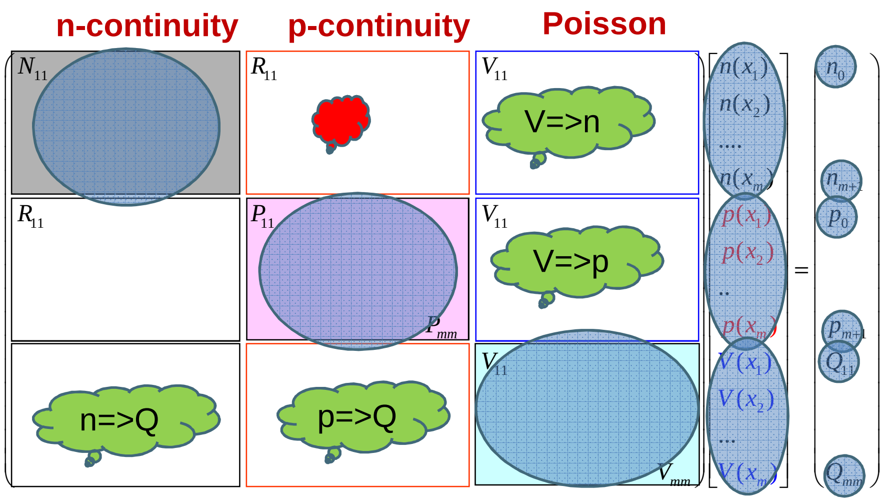
Dopant density

$$V = V_A$$

One could have unequal materials on the two contact sides, one must be careful to use the right intrinsic concentration <-> material.

$$V = 0$$

Numerical Solution…



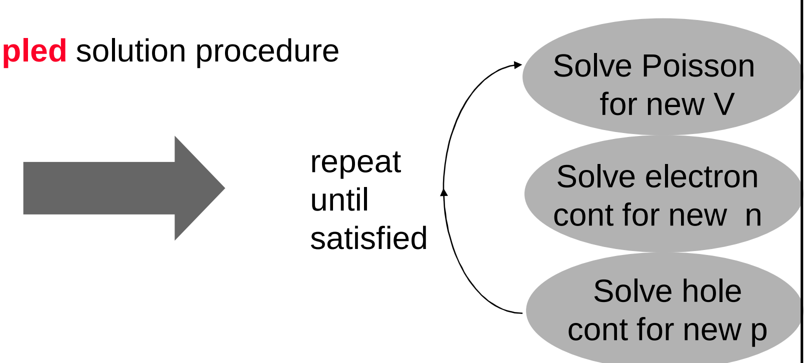
Off-diagonal terms are Poisson-Continuity equations talking to each other. Recombination-generation terms also feed into continuity equations.

3) Uncoupled Numerical Solution

The semiconductor equations are nonlinear!
(but they are linear individually)

Guess V,n,p

Uncoupled solution procedure



Summary

1) Two methods to solve drift-diffusion equation consistently – analytical and numerical.

2) Analytical solution provides great insight and the solution methodology is similar to that of Schrodinger equations.

3) Numerical solution is more versatile. One begins with a set of equations and boundary conditions, discretize the equations on a grid with N nodes to obtain 3N nonlinear equations in 3N unknowns, and solve the system of nonlinear equations by iteration.