Lecture8

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Residue and Jacobian matrix

- In silicon regions, consider the integrated Poisson equation.
  - The i-th entry of the residue vector reads

$$r_i = \frac{\epsilon_{si}}{\Delta x}(\phi_{i+1} - 2\phi_i + \phi_{i-1}) - (\Delta x) q N_{acc} - (\Delta x) q n_i \exp\left(\frac{q\phi_i}{k_B T}\right)$$

  - The i-th row of the Jacobian matrix reads

$$J_{i,i+1} = \frac{\epsilon_{si}}{\Delta x}$$

$$J_{i,i} = -2\frac{\epsilon_{si}}{\Delta x} - (\Delta x) q n_i \frac{q}{k_B T} \exp\left(\frac{q\phi_i}{k_B T}\right)$$

$$J_{i,i-1} = \frac{\epsilon_{si}}{\Delta x}$$

MATLAB example (1)

- Defining variables

```
q = 1.602192e-19; % Elementary charge, C
eps0 = 8.854187817e-12; % Vacuum permittivity, F/m
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
thermal = k_B*T/q; % Thermal voltage, V
Deltax = 0.1e-9; % 0.1 nm spacing
N = 61; % 6 nm thick
x = Deltax*transpose([0:N-1]); % real space, m
interface1 = 6; % At x=0.5 nm
interface2 = 56; % At x=5.5 nm
eps_si = 11.7; eps_ox = 3.9; % Relative permittivity
Nacc = 1e24; % 1e18 /cm^3
ni = 1.075e16; % 1.075e10 /cm^3
coef = Deltax*Deltax*q/eps0;
```

MATLAB example (2)

- `Jaco` and `res` should be constructed.
  - Boundary conditions

```
res = zeros(N,1);
Jaco = sparse(N,N);
res(1,1) = phi(1,1) - 0.33374;
Jaco(1,1) = 1.0;
res(N,1) = phi(N,1) - 0.33374;
Jaco(N,N) = 1.0;
```

MATLAB example (3)

- Laplacian part

```
for ii=2:N-1
   if     (ii< interface1 || ii> interface2)
      res(ii,1) = eps_ox*phi(ii+1,1) - 2*eps_ox*phi(ii,1) + eps_ox*phi(ii-1,1);
      Jaco(ii,ii-1) = eps_ox; Jaco(ii,ii) = -2*eps_ox;        Jaco(ii,ii+1) = eps_ox;
   elseif (ii==interface1)
      res(ii,1) = eps_si*phi(ii+1,1) - (eps_si+eps_ox)*phi(ii,1) + eps_ox*phi(ii-1,1);
      Jaco(ii,ii-1) = eps_ox; Jaco(ii,ii) = -(eps_si+eps_ox); Jaco(ii,ii+1) = eps_si;
   elseif (ii==interface2)
      res(ii,1) = eps_ox*phi(ii+1,1) - (eps_ox+eps_si)*phi(ii,1) + eps_si*phi(ii-1,1);
      Jaco(ii,ii-1) = eps_si; Jaco(ii,ii) = -(eps_ox+eps_si); Jaco(ii,ii+1) = eps_ox;
   else
      res(ii,1) = eps_si*phi(ii+1,1) - 2*eps_si*phi(ii,1) + eps_si*phi(ii-1,1);
      Jaco(ii,ii-1) = eps_si; Jaco(ii,ii) = -2*eps_si;        Jaco(ii,ii+1) = eps_si;
   end
end
```

MATLAB example (4)

- Charge part

```
for ii=interface1:interface2
   if     (ii==interface1)
      res(ii,1) = res(ii,1) - coef*(Nacc+ni*exp(phi(ii,1)/thermal))*0.5;
      Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal*0.5;
   elseif (ii==interface2)
      res(ii,1) = res(ii,1) - coef*(Nacc+ni*exp(phi(ii,1)/thermal))*0.5;
      Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal*0.5;
   else
      res(ii,1) = res(ii,1) - coef*(Nacc+ni*exp(phi(ii,1)/thermal));
      Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal;
   end
end
```

MATLAB example (5)

- Full code

```
(Defining variables. Copy-and-paste)
phi = zeros(N,1);
phi(:,1) = 0.33374;
for newton=1:10
    (Jaco and res are constructed here. Copy-and-paste)
    update = Jaco \ (-res);
    phi = phi + update;
end
plot(x,phi);
```

Homework#8

- Due: AM08:00, October 5 (Next Monday)
- Problem#1
  - Write the nonlinear Poisson solver for the double-gate structure.
  - The oxide thickness is 0.8 nm.
  - Calculate the integrated electron density (/cm^2) as a function of the gate voltage. (You must use the self-consistent solution.)
  - Suggested voltage range: From 0 V to 1 V