MOS Capacitor Simulation project

1 Equations

$$J_n = q\mu_n nE + qD_n \frac{dn}{dx} \tag{1}$$

$$V_t = \frac{KT}{q} \tag{2}$$

$$\phi = \frac{V}{V_t} \tag{3}$$

$$E = -\frac{dV}{dx} \tag{4}$$

$$\implies J_n = KT\mu_n \left(\frac{nE}{V_t} + \frac{dn}{dx}\right) = KT\mu_n \left(\frac{-nd\phi}{dx} + \frac{dn}{dx}\right) \tag{5}$$

$$\text{Carrier continuity equation:} \frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n - R_n \tag{6}$$

$$= \frac{1}{q}\frac{\partial J_n}{\partial x} - \frac{n - n_o}{\tau_n} \tag{7}$$

Before proceeding forward, it is necessary to realize that the current is essentially a quantity that is defined as a flux that goes from one point to another. Therefore, it is defined between two nodes, as the flux that enters the node. Defining current at a particular point does not carry significant meaning. So, now that we have understood the meaning of current, we define it as the flux flowing between node $i-1$ and node i. In order to uniquely represent the flux between these nodes, we will use the index $i-\frac{1}{2}$ to denote the element between nodes $i-1$ and i. Similarly, to represent the element between node i and node $i+1$, we will use the index $i+\frac{1}{2}$. Let us assume $n(x) = u(x)\, e^{\phi(x)}$. This is because the carrier concentration depends exponentially on the potential. Also we assume potential to be linear between any two nodes. So,

$$\phi = \phi_{i-1} + \frac{\phi_i - \phi_{i+1}}{x_i - x_{i-1}}(x - x_{i-1}) = \phi_{i-1} + \frac{\phi_i - \phi_{i-1}}{\Delta x_{i-1}}(x - x_{i-1}) \tag{8}$$

$$\implies J_{i-\frac{1}{2}} = kT\mu_n e^{\phi}\frac{du}{dx} \tag{9}$$

$$\implies \int_{x_{i-1}}^{x_i} J_{i-\frac{1}{2}} e^{-\phi}\, dx = \int_{u_{i-1}}^{u_i} kT\mu_n\, du \tag{10}$$

$$\implies J_{i-\frac{1}{2}} = \frac{KT\mu_n}{\Delta x_{i-1}}\left(\frac{n_i - n_{i-1}e^{(\phi_i - \phi_{i-1})}}{e^{\phi_i - \phi_{i-1}} - 1}\right)(\phi_i - \phi_{i-1}) \tag{11}$$

$$\text{Bernoulli function: } B(x) = \frac{x}{e^x - 1} \tag{12}$$

$$\implies J_{i-\frac{1}{2}} = \frac{KT\mu_n}{\Delta x_{i-1}} B(\phi_i - \phi_{i-1})\left(n_i - n_{i-1}e^{(\phi_i - \phi_{i-1})}\right) \tag{13}$$

$$J_{i+\frac{1}{2}} = \frac{KT\mu_n}{\Delta x_i} B(\phi_{i+1} - \phi_i)\left(n_{i+1} - n_i e^{(\phi_{i+1} - \phi_i)}\right) \tag{14}$$

Since, in DC bias, steady state we have $\frac{dJ}{dx} = 0$ and assuming $\Delta x_i = x_{i+1} - x_i = ab^i$. So,

$$J_{1-\frac{1}{2}} = J_{1+\frac{1}{2}} \tag{15}$$

$$\implies bB(\phi_i - \phi_{i-1})\left(n_i - n_{i-1}e^{(\phi_i - \phi_{i-1})}\right) = B(\phi_{i+1} - \phi_i)\left(n_{i+1} - n_i e^{(\phi_{i+1} - \phi_i)}\right) \tag{16}$$

$$\implies \alpha_{i-1}n_{i-1} + \alpha_i n_i + \alpha_{i+1}n_{i+1} = 0 \quad \forall \quad i \geq 1 \tag{17}$$

$$\alpha_{i-1} = bB(\phi_i - \phi_{i-1})e^{(\phi_i - \phi_{i-1})} \tag{18}$$

$$\alpha_i = -\left(bB(\phi_i - \phi_{i-1}) + B(\phi_{i+1} - \phi_i)e^{(\phi_{i+1} - \phi_i)}\right) \tag{19}$$

$$\alpha_{i+1} = B(\phi_{i+1} - \phi_i) \tag{20}$$

Similarly for p, assume $p(x) = u(x)e^{-\phi(x)}$, so we get

$$\beta_{i-1}p_{i-1} + \beta_i p_i + \beta_{i+1}p_{i+1} = 0 \quad \forall \quad i \geq 1 \tag{21}$$

$$\beta_{i-1} = bB(\phi_i - \phi_{i-1}) \tag{22}$$

$$\beta_i = -\left(bB(\phi_{i+1} - \phi_i) + bB(\phi_{i+1} - \phi_i)e^{(\phi_i - \phi_{i-1})}\right) \tag{23}$$

$$\beta_{i+1} = B(\phi_{i+1} - \phi_i)e^{(\phi_{i+1} - \phi_i)} \tag{24}$$

Now, when we apply AC signal along with DC bias,

$$\frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} - \frac{n - n_o}{\tau_n} \tag{25}$$

$$\frac{n_i(t+\Delta t) - n_i(t)}{\Delta t} = \frac{1}{q}\frac{J_{i+\frac{1}{2}}(t+\Delta t) - J_{i-\frac{1}{2}}(t+\Delta t)}{\Delta x_{i-\frac{1}{2}}} - \frac{n_i(t+\Delta t) - n_i(t=0)}{\tau_n} \tag{26}$$

$$J_{i-\frac{1}{2}}(t+\Delta t) = \frac{KT\mu_n}{\Delta x_{i-1}} B\left(\phi_i(t+\Delta t) - \phi_{i-1}(t+\Delta t)\right)\left[n_i(t+\Delta t) - n_{i-1}(t+\Delta t) e^{\phi_i(t+\Delta t) - \phi_{i-1}(t+\Delta t)}\right] \tag{27}$$

$$J_{i+\frac{1}{2}}(t+\Delta t) = \frac{KT\mu_n}{\Delta x_i} B\left(\phi_{i+1}(t+\Delta t) - \phi_i(t+\Delta t)\right)\left[n_{i+1}(t+\Delta t) - n_i(t+\Delta t) e^{\phi_{i+1}(t+\Delta t) - \phi_i(t+\Delta t)}\right] \tag{28}$$

$$\alpha_{i-1} n_{i-1}(t+\Delta t) + \alpha_i n_i(t+\Delta t) + \alpha_{i+1}(t+\Delta t) n_{i+1} = -\frac{n_i(t)}{\Delta t} - \frac{n_i(t=0)}{\tau_n} \quad \forall \quad i \geq 1 \tag{29}$$

$$\alpha_{i-1} = \frac{V_t\mu_n}{\Delta x_{i-1}\Delta x_{i-\frac{1}{2}}} B(\phi_i - \phi_{i-1}) e^{(\phi_i - \phi_{i-1})} = \frac{b^{\frac{3}{2}} V_t\mu_n}{\Delta x_i^{\,2}} B(\phi_i - \phi_{i-1}) e^{(\phi_i - \phi_{i-1})} \tag{30}$$

$$\alpha_i = -\left(\frac{V_t\mu_n}{\Delta x_{i-\frac{1}{2}}}\left(\frac{B(\phi_i - \phi_{i-1})}{\Delta x_{i-1}} + \frac{B(\phi_{i+1} - \phi_i) e^{(\phi_{i+1} - \phi_i)}}{\Delta x}\right) + \left(\frac{1}{\Delta t} + \frac{1}{\tau_n}\right)\right) \tag{31}$$

$$= -\left(\frac{\sqrt{b} V_t\mu_n}{\Delta x_i^{\,2}}\left(b B(\phi_i - \phi_{i-1}) + B(\phi_{i+1} - \phi_i) e^{(\phi_{i+1} - \phi_i)}\right) + \left(\frac{1}{\Delta t} + \frac{1}{\tau_n}\right)\right) \tag{32}$$

$$\alpha_{i+1} = \frac{V_t\mu_n}{\Delta x_i \Delta x_{i-\frac{1}{2}}} B(\phi_{i+1} - \phi_i) = \frac{\sqrt{b} V_t\mu_n}{\Delta x_i^{\,2}} B(\phi_{i+1} - \phi_i) \tag{33}$$

Similarly for p we get,

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\frac{\partial J_p}{\partial x} - \frac{p - p_o}{\tau_p} \tag{34}$$

$$\frac{p_i(t+\Delta t) - p_i(t)}{\Delta t} = -\frac{1}{q}\frac{J_{i+\frac{1}{2}}(t+\Delta t) - J_{i-\frac{1}{2}}(t+\Delta t)}{\Delta x_{i-\frac{1}{2}}} - \frac{p_i(t+\Delta t) - p_i(t=0)}{\tau_p} \tag{35}$$

$$J_{i-\frac{1}{2}}(t+\Delta t) = \frac{KT\mu_p}{\Delta x_{i-1}} B\left(\phi_i(t+\Delta t) - \phi_{i-1}(t+\Delta t)\right)\left[p_i(t+\Delta t) e^{\phi_i(t+\Delta t) - \phi_{i-1}(t+\Delta t)} - p_{i-1}(t+\Delta t)\right] \tag{36}$$

$$J_{i+\frac{1}{2}}(t+\Delta t) = \frac{KT\mu_p}{\Delta x_i} B\left(\phi_{i+1}(t+\Delta t) - \phi_i(t+\Delta t)\right)\left[p_{i+1}(t+\Delta t) e^{\phi_{i+1}(t+\Delta t) - \phi_i(t+\Delta t)} - p_i(t+\Delta t)\right] \tag{37}$$

$$\beta_{i-1} p_{i-1} + \beta_i p_i + \beta_{i+1} p_{i+1} = \frac{p_i(t)}{\Delta t} + \frac{p_i(t=0)}{\tau_p} \quad \forall \quad i \geq 1 \tag{38}$$

$$\tag{39}$$

$$\beta_{i-1} = \frac{V_t \mu_p}{\Delta x_{i-1} \Delta x_{i-\frac{1}{2}}} B(\phi_i - \phi_{i-1}) = \frac{b^{\frac{3}{2}} V_t \mu_n}{\Delta {x_i}^2} B(\phi_i - \phi_{i-1}) \tag{40}$$

$$\beta_i = -\left(\frac{V_t \mu_p}{\Delta x_{i-\frac{1}{2}}} \left(\frac{B(\phi_i - \phi_{i-1}) e^{(\phi_i - \phi_{i-1})}}{\Delta x_{i-1}} + \frac{B(\phi_{i+1} - \phi_i)}{\Delta x} \right) - \left(\frac{1}{\Delta t} + \frac{1}{\tau_p} \right) \right) \tag{41}$$

$$= -\left(\frac{\sqrt{b} V_t \mu_p}{\Delta {x_i}^2} \left(b B(\phi_i - \phi_{i-1}) e^{(\phi_i - \phi_{i-1})} + B(\phi_{i+1} - \phi_i) \right) - \left(\frac{1}{\Delta t} + \frac{1}{\tau_p} \right) \right) \tag{42}$$

$$\beta_{i+1} = \frac{V_t \mu_p}{\Delta x_i \Delta x_{i-\frac{1}{2}}} B(\phi_{i+1} - \phi_i) e^{(\phi_{i+1} - \phi_i)} = \frac{\sqrt{b} V_t \mu_n}{\Delta {x_i}^2} B(\phi_{i+1} - \phi_i) e^{(\phi_{i+1} - \phi_i)} \tag{43}$$

In DC steady state, (no AC signal given), we can use (44) and (45).

$$n = N_c \frac{2}{\sqrt{\pi}} F_{\frac{1}{2}} \left[\frac{V - V_f}{V_t} \right] \tag{44}$$

$$p = N_v \frac{2}{\sqrt{\pi}} F_{\frac{1}{2}} \left[\frac{V_f - V + V_g}{V_t} \right] \tag{45}$$

$$V_g = \frac{-E_g}{q} \tag{46}$$

$$V_t = \frac{kT}{q} \tag{47}$$

$$\rho(x_i, t_i) = N_D - N_A + p(x_i, t_i) - n(x_i, t_i) \tag{48}$$

Far inside the bulk, $V = 0, \rho = 0$, we can get V_f from this.

$$N_c F_{\frac{1}{2}} \left[\frac{-V_f}{V_t} \right] - N_v F_{\frac{1}{2}} \left[\frac{V_f + V_g}{V_t} \right] = \frac{\sqrt{\pi}}{2} (N_D - N_A) \tag{49}$$

So to get n_s, p_s, just substitute $V = V_s$ in (44) and (45).
To get n_s, p_s when AC signal is applied, assuming DC component of n_s is already known at a particular surface potential V_s, we can linearize n_s around this point for small changes in V_s by differentiating with respect to V_s:

$$\frac{\partial n_s}{\partial V_s} = \frac{\partial}{\partial V_s} \left(N_c \frac{2}{\sqrt{\pi}} F_{\frac{1}{2}} \left[\frac{V_s - V_f}{V_t} \right] \right) \tag{50}$$

$$= N_c \frac{2}{\sqrt{\pi}} \frac{\partial}{\partial V_s} \left(F_{\frac{1}{2}} \left[\frac{V_s - V_f}{V_t} \right] \right) \tag{51}$$

The Fermi-Dirac integral of order j is defined as:

$$F_j(\eta) = \int_0^\infty \frac{x^j}{1+e^{x-\eta}}\,dx \tag{52}$$

$$\frac{dF_j(\eta)}{d\eta} = \frac{d}{d\eta}\int_0^\infty \frac{x^j}{1+e^{x-\eta}}\,dx \tag{53}$$

$$\frac{dF_j(\eta)}{d\eta} = \int_0^\infty \frac{\partial}{\partial\eta}\left(\frac{x^j}{1+e^{x-\eta}}\right)dx \tag{54}$$

$$\frac{\partial}{\partial\eta}\frac{x^j}{1+e^{x-\eta}} = x^j\cdot\frac{e^{x-\eta}}{(1+e^{x-\eta})^2} \tag{55}$$

$$\frac{\partial}{\partial x}\left(\frac{1}{1+e^{x-\eta}}\right) = -\frac{e^{x-\eta}}{(1+e^{x-\eta})^2} \tag{56}$$

$$\implies \frac{dF_j(\eta)}{d\eta} = -\int_0^\infty x^j\cdot\frac{d}{dx}\left(\frac{1}{1+e^{x-\eta}}\right)dx \tag{57}$$

We apply integration by parts with $u = x^j$ and $dv = \frac{d}{dx}\left(\frac{1}{1+e^{x-\eta}}\right)dx$, giving:

$$\frac{dF_j(\eta)}{d\eta} = \left[x^j\cdot -\frac{1}{1+e^{x-\eta}}\right]_0^\infty + \int_0^\infty jx^{j-1}\cdot\frac{1}{1+e^{x-\eta}}\,dx \tag{58}$$

$$= j\int_0^\infty x^{j-1}\cdot\frac{1}{1+e^{x-\eta}}\,dx \tag{59}$$

$$= j\cdot F_{j-1}(\eta) \tag{60}$$

$$\implies \frac{\partial F_{\frac{1}{2}}\left[\frac{V_s-V_f}{V_t}\right]}{\partial V_s} = \frac{1}{2V_t}F_{\frac{-1}{2}}\left[\frac{V_s-V_f}{V_t}\right] \tag{61}$$

$$\implies \frac{\partial n_s}{\partial V_s} = \frac{N_c}{\sqrt{\pi}V_t}F_{\frac{-1}{2}}\left[\frac{V_s-V_f}{V_t}\right] \tag{62}$$

$$\implies n_s(t+\Delta t) - n_s(t) = \frac{N_c}{\sqrt{\pi}V_t}F_{\frac{-1}{2}}\left[\frac{V_s-V_f}{V_t}\right](V_s(t+\Delta t)-V_s(t)) \tag{63}$$

$$p_s(t+\Delta t) - p_s(t) = -\frac{N_v}{\sqrt{\pi}V_t}F_{\frac{-1}{2}}\left[\frac{V_g+V_f-V_s}{V_t}\right](V_s(t+\Delta t)-V_s(t)) \tag{64}$$

$$Q = \epsilon_{ox}\mathcal{E}_{ox} \tag{65}$$

$$C = \frac{dQ}{dV_G} = \epsilon_{ox}\frac{\frac{d\mathcal{E}_{ox}}{dt}}{\frac{dV_G}{dt}} \tag{66}$$

$$= \epsilon_{ox}\frac{\mathcal{E}_{ox}(t_{i+1}) - \mathcal{E}_{ox}(t_i)}{V_G(t_{i+1}) - V_G(t_i)} \tag{67}$$

$$= \epsilon_{ox}\frac{(V(0,t_{i+1}) - V(x_1,t_{i+1})) - (V(0,t_i) - V(x_1,t_i))}{(V_G(t_{i+1}) - V_G(t_i))\,\Delta x_1} \tag{68}$$

$$= \frac{\epsilon_{ox}}{\Delta x_1}\left(1 - \frac{V(x_1,t_{i+1}) - V(x_1,t_i)}{V_G(t_{i+1}) - V_G(t_i)}\right) \tag{69}$$

2 To Do

1. Proper meshing. Make sure this meshing can give accurate and simple results while differentiation as we write difference equations.
2. Verify all the equations, boundary conditions and validity of these in which conditions. For example mobility is dependent on temperature and doping concentrations. Similarly check for other things.
3. Poisson Equation
   - $F(V_{i-1}, V_i, V_{i+1}) = 0, J\Delta V = -F$. Get ΔV.
   - From ΔV get V.
4. Carrier Concentration
   - Solve for DC bias to get n($t = 0$) using Scharfetter-Gummel Discretization. You'll get $\alpha_{i-1}n_{i-1} + \alpha_i n_i + \alpha_{i+1}n_{i+1} = 0$.
   - Solve for $t + \Delta t$ now. Get $n(t + \Delta t)$. You'll get

     $$\alpha_{i-1}n_{i-1} + \alpha_i n_i + \alpha_{i+1}n_{i+1} = -\left(\frac{n_i(t)}{\Delta t} + \frac{n_i(t = 0)}{\tau_n}\right)$$

     Solve for t=0 to get at next time point.
   - Similarly solve for p.
   - Then calculate C from it.
5. Write main code, self-consistent code. This involves controlling various parameters, saving files for equilibrium, steady state and ac analysis and then saving C-VG data.
6. Write python codes to plot conc-x, voltage-x, C-VG graphs. (conc-x, voltage-x for debugging, C-VG is the actual one needed).
7. Write a makefile to run required the files.