Hydrodynamic Modeling: Hydrodynamic Equations

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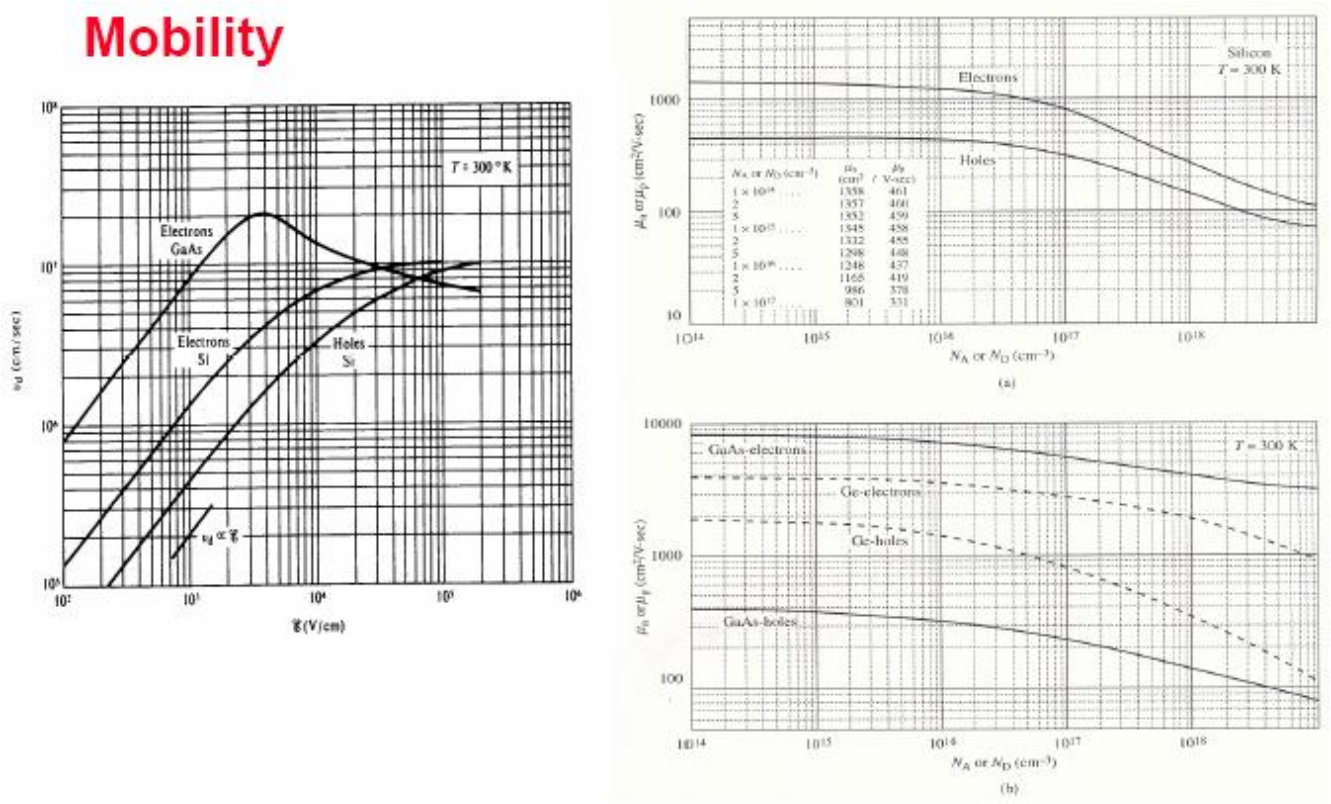
Drift-Diffusion Approaches

- Valid when diffusive transport dominates

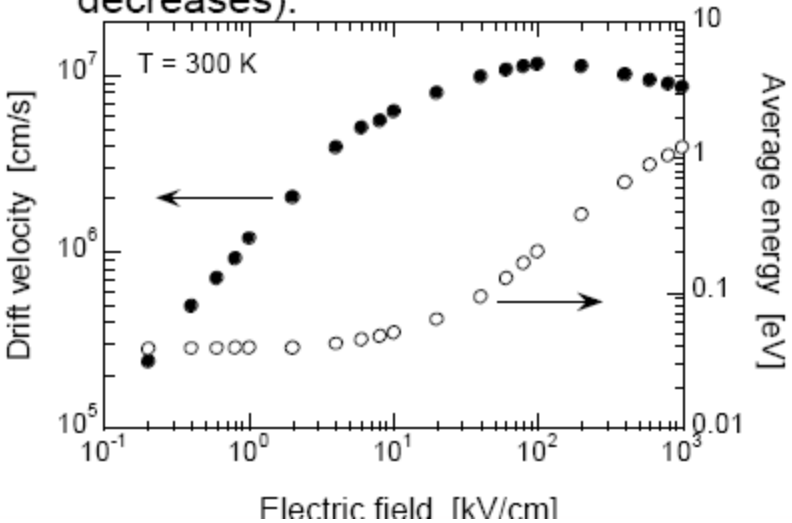


John D. Cressler

after Pierret, Semiconductor Device Fundamentals, 1996

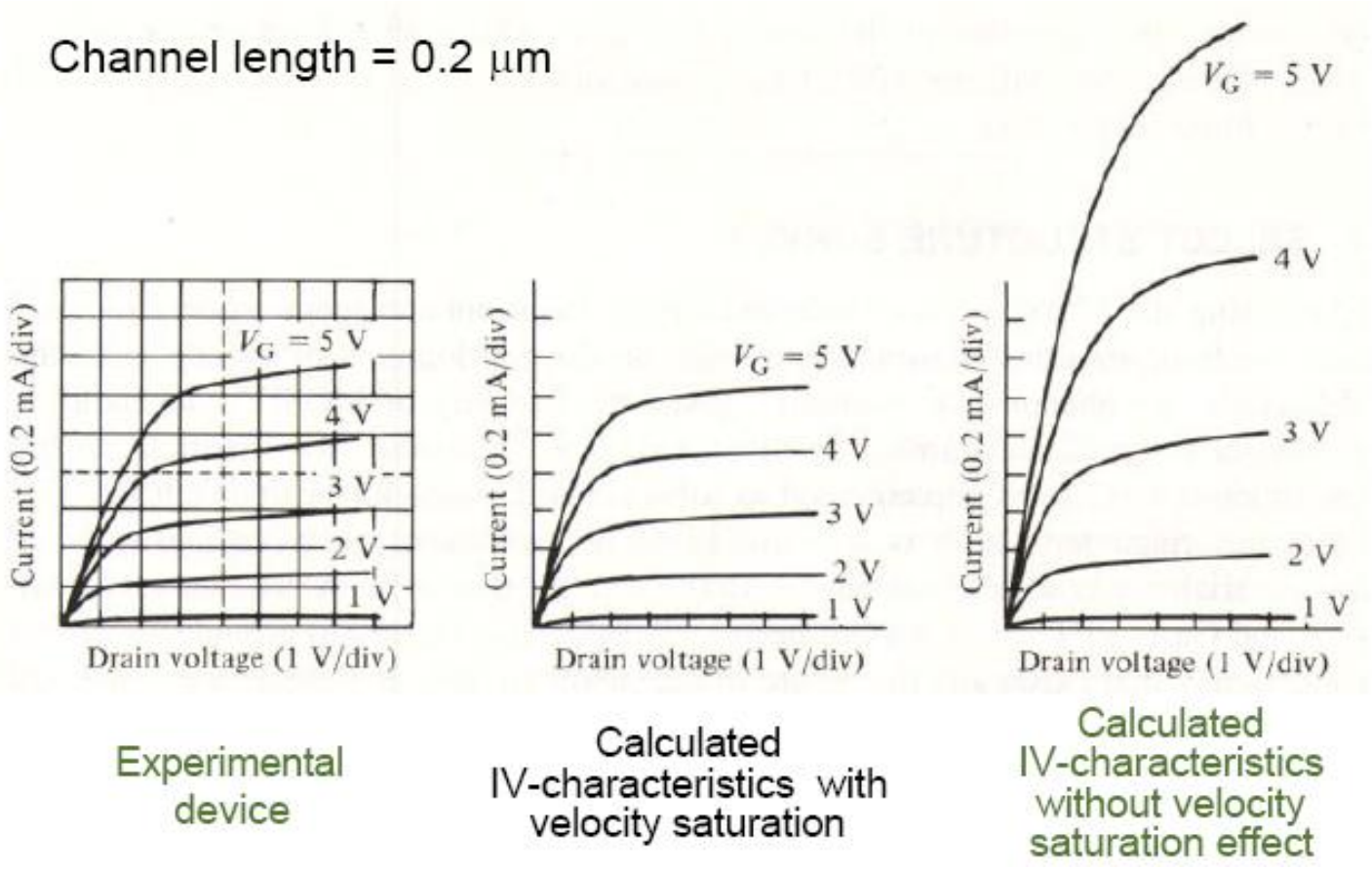
Extension of DD Aproaches Validity

- Introduction of the field-dependent mobility
  - Long-channel devices → *ID-VD* curves nearly constant in saturation
  - Short-channel device → Electric fields become very high and the drift-velocity becomes constant (mobility decreases).



Drift velocity and average electron energies for bulk *Si*

Velocity Saturation Implications



Velocity Saturation

- A simplified expression is obtained using:

$$I_D = -qA_{eff}nv_d, \quad A_{eff} = Zy_{eff}$$

Device width; Effective thickness of the inversion layer

i.e. the velocity-limited drain current equals to:

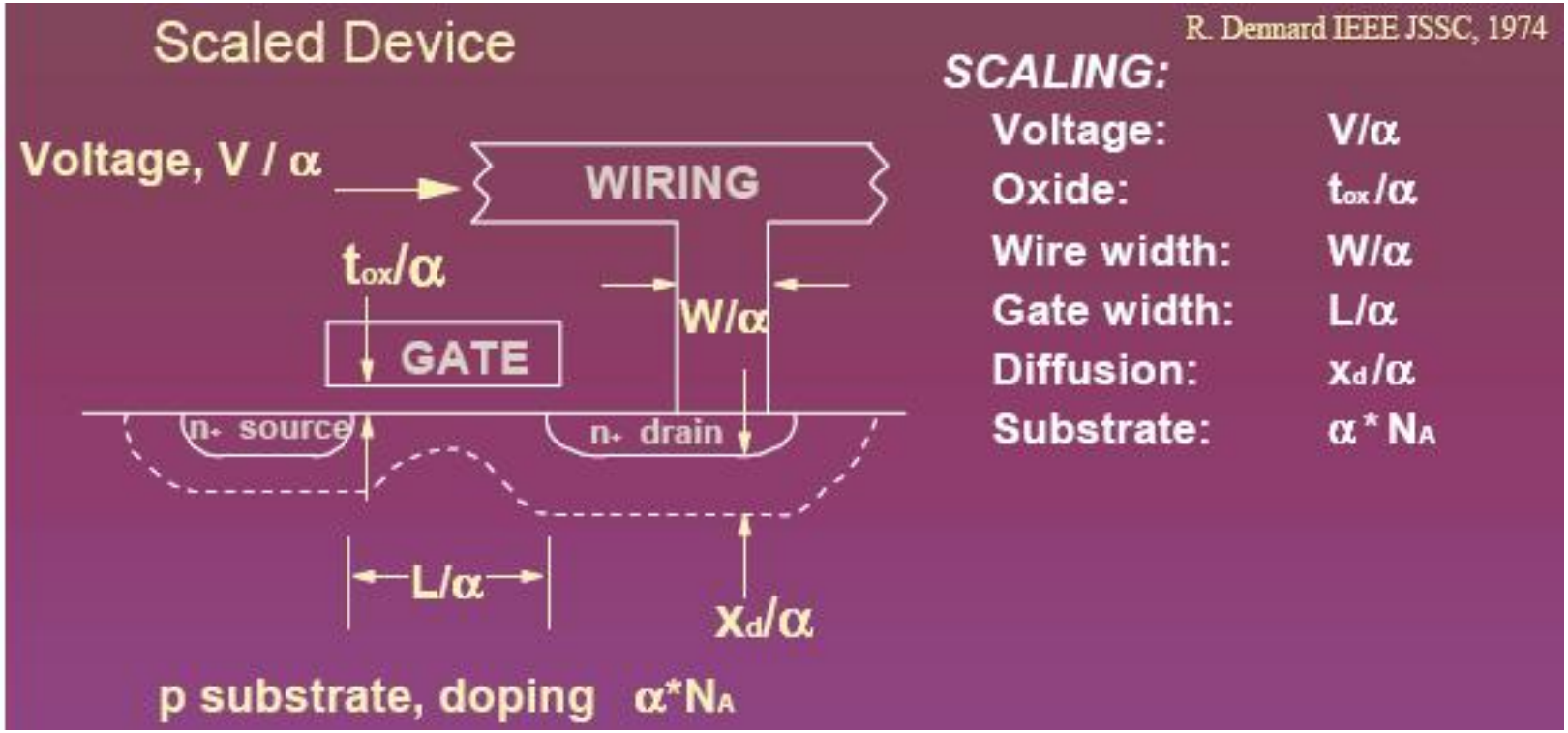
$$I_D = -qZy_{eff}nv_d = \underbrace{-qy_{eff}n}_{Q_N} Zv_d = Zv_d C_{ox}(V_G - V_T)$$

- Comparing the above expression with the mobility-limited one for a long-channel device, we get:

$$v_{sat} \leftrightarrow \frac{\mu_{eff}(V_G - V_T)}{2L}$$

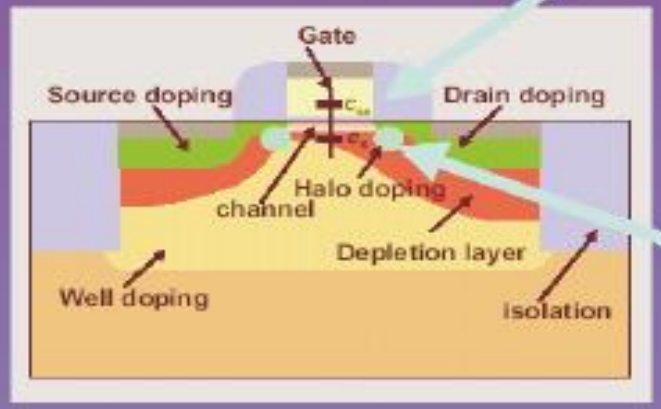
For V_G-V_T=5 V we get L =1.25 μm (v_{sat} = 10^7 cm/s)

Device Scaling



Challenges in Scaled Devices

Threshold voltage:
- kT/q (subthreshold slope)
- V_{DD} - V_T decreases



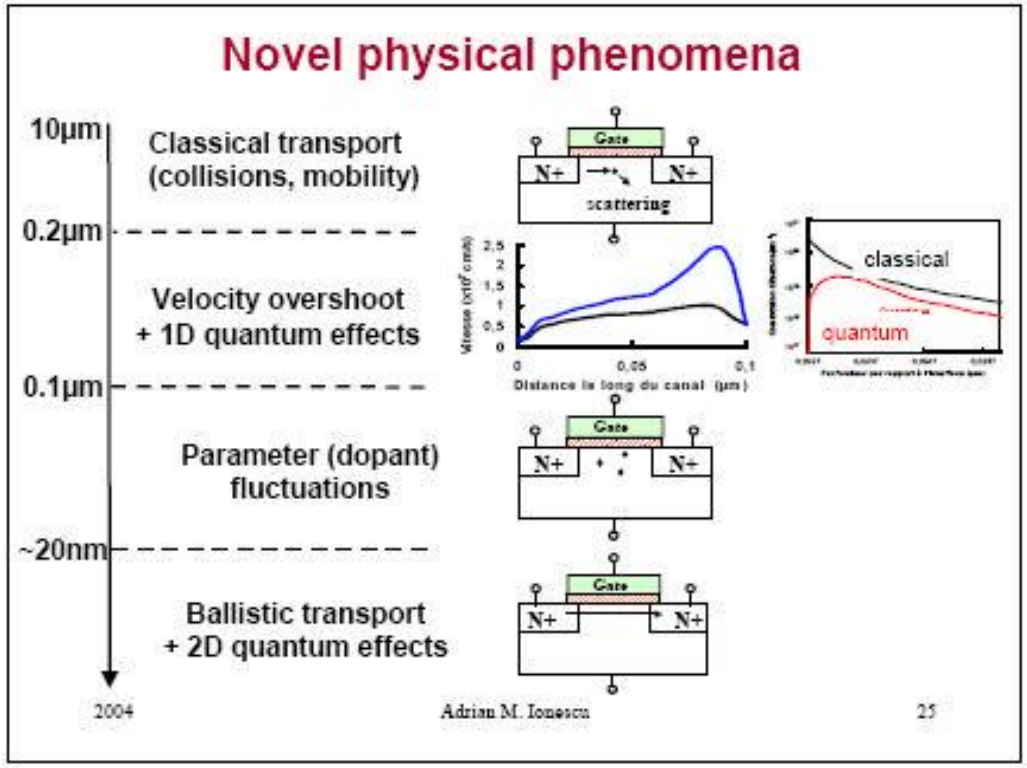
Gate:
- tunneling
- inversion layer
- polySi gate depletion, activation, dopant penetration

Tunneling:
- drain to body
- source to drain

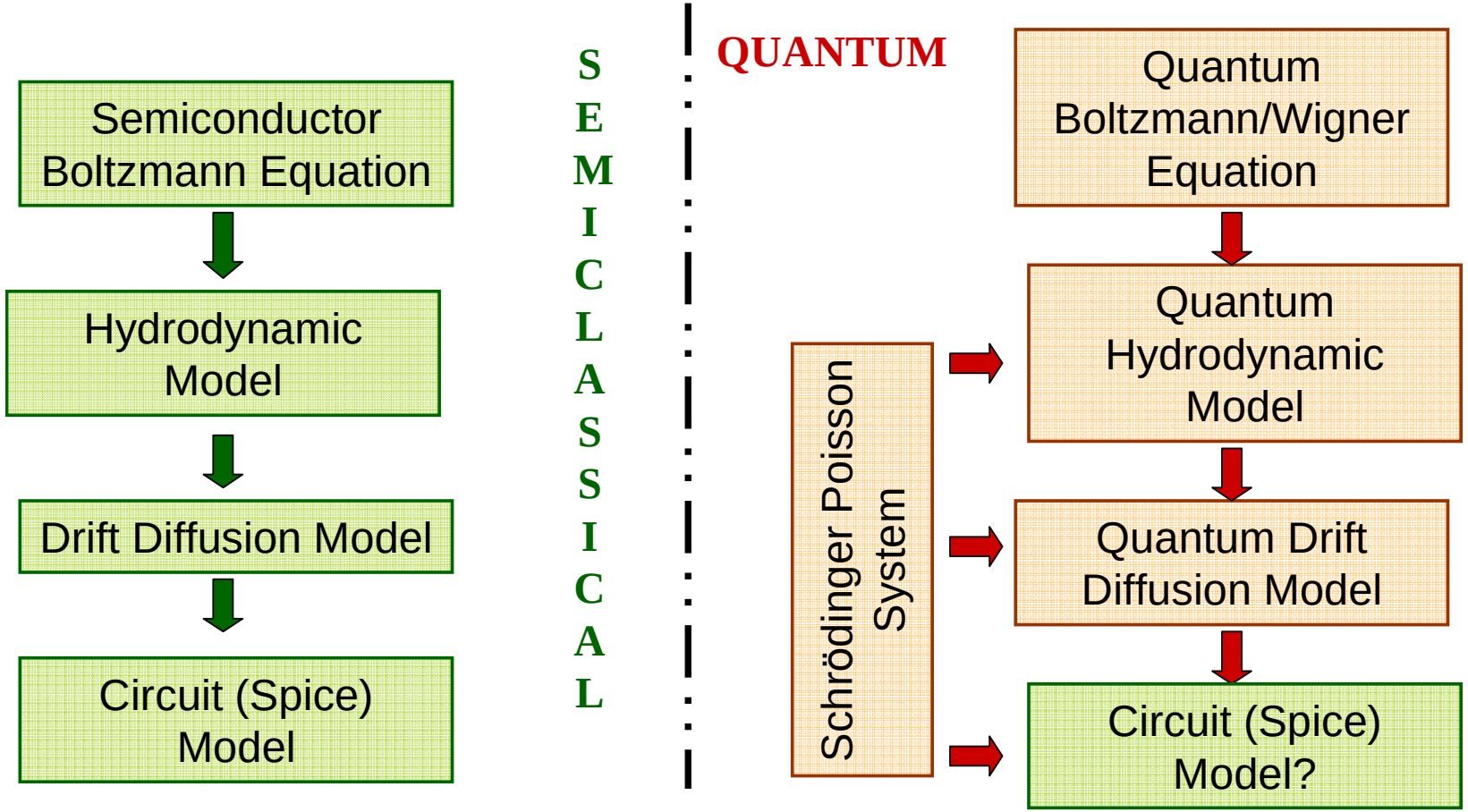
Dopant profile control:
- transient enhanced diffusion
- ion implantation
- RTA ramp rate limitation
- discrete, random dopant placement

High electric fields:
- mobility degradation
- reliability

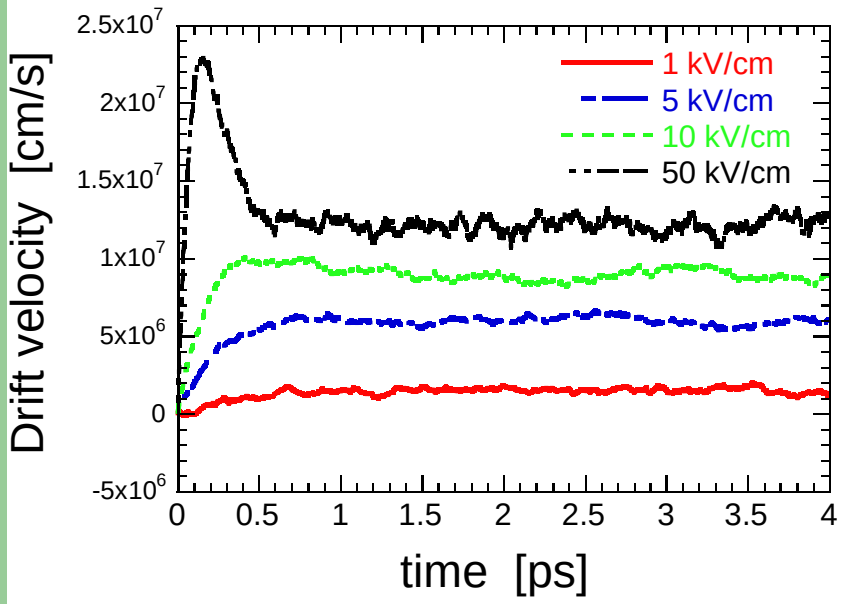
Length Scales Over Which These Effects Occur



Modeling Hierarchy

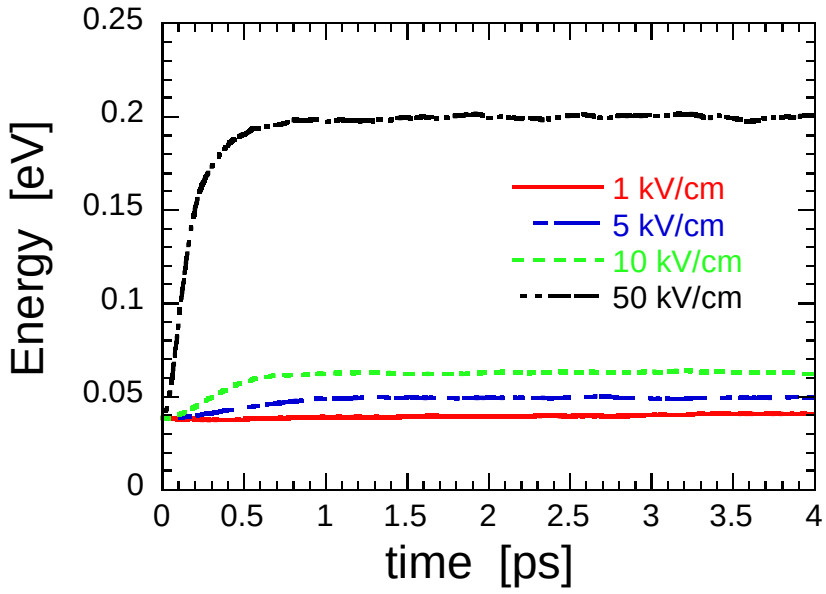


Velocity Overshoot in Bulk Si



Time evolution of mean drift velocity. Electric field is: (a) 1.0 kV/cm, (b) 5.0 kV/cm, (c) 10 kV/cm, and (d) 50 kV/cm, respectively.

Time evolution of the average electron kinetic energy. The electric field equals: (a) 1 kV/cm, (b) 5 kV/cm, (c) 10 kV/cm, and (d) 50 kV/cm, respectively.



Velocity Overshoot

- We can describe the motion of the electrons between collisions by simple Newton's Law:

$$m^* \frac{dv_{dx}}{dt} = -qF_x$$

- In a simplified approach (momentum balance equation for an average carrier) that neglects diffusion, we have

$$m^* \frac{dv_{dx}}{dt} = -qF_x - \frac{m^* v_{dx}}{\tau_m}$$

- For a uniform electric field applied at t=0, the solution of the above equation is of the form:

$$v_{dx}(t) = \frac{q\tau_m}{m^*} F_x \left[e^{-t/\tau_m} - 1 \right]$$

Velocity Overshoot, Cont'd

- When steady state has been reached, the electrons have traveled the distance:

$$d = \int_0^{\tau_m} v_{dx}(t)dt = \frac{q\tau_m^2}{em^*}Fx$$

- For F_x = 10kV/cm, we have that:

  ? d » 200Å for electrons in Si

- Why do we observe velocity overshoot?
  1. The energy relaxation time is larger than momentum relaxation time
  2. At first, the electric field simply displaces the distribution function with little change on its shape

Velocity Overshoot, Cont'd

3. Later on, collisions broaden the distribution, the electron temperature increases and drift velocity drops.

- Velocity overshoot effect reduces the electron transit time, i.e. leads to faster devices.

Hydrodynamic Simulator

- Basic hydrodynamic equations
- Ensemble relaxation rates and their calculation
- Discretization of the balance or hydrodynamic equations

Basic Hydrodynamic Equations

- To derive the Balance Equations, one starts with the BTE , multiplies it with an appropriate function $\phi(\mathbf{k})$ and integrates over **k** to get:

$$\frac{\partial \Phi}{\partial t} = -\nabla_{\mathbf{r}} \cdot J_{\phi} + G_{\phi} - R_{\phi}$$

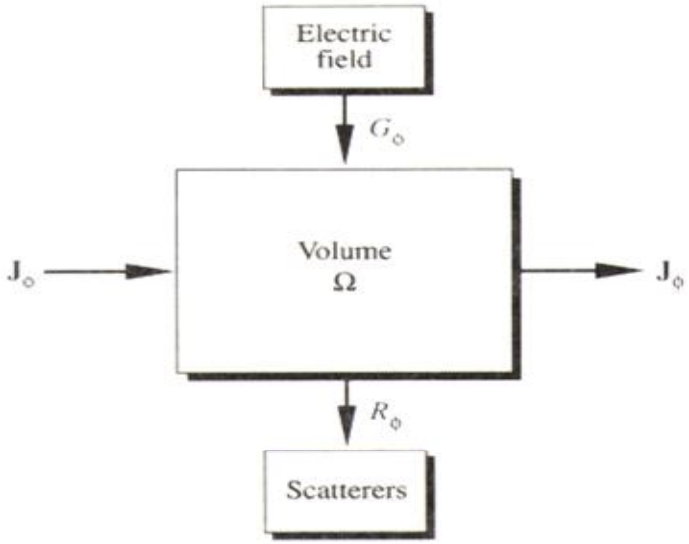
where:

$$\Phi(\mathbf{r},t) = \int d\mathbf{p}\,\phi(\mathbf{p}) f(\mathbf{r},\mathbf{p},t)$$

$$J_{\phi}(\mathbf{r},t) = \int d\mathbf{p}\,\phi(\mathbf{p}) v(\mathbf{p}) f(\mathbf{r},\mathbf{p},t)$$

$$G_{\phi}(\mathbf{r},t) = -e\mathbf{E} \cdot \int d\mathbf{p} \left(\nabla_{\mathbf{p}} \phi\right) f(\mathbf{r},\mathbf{p},t)$$

$$R_{\phi}(\mathbf{r},t) = -\int d\mathbf{p}\,\phi(\mathbf{p}) \left.\frac{\partial f}{\partial t}\right|_{coll}$$



Carrier Density

- Balance equation for the carrier density is obtained by assuming that $\phi(\mathbf{p})=1$: $\Phi(\mathbf{r},t) = n(\mathbf{r},t)$

$$\mathbf{J}_\phi(\mathbf{r},t) = \int d\mathbf{p}\mathbf{v}(\mathbf{p}) f(\mathbf{r},\mathbf{p},t) = -\frac{J_n}{e}$$

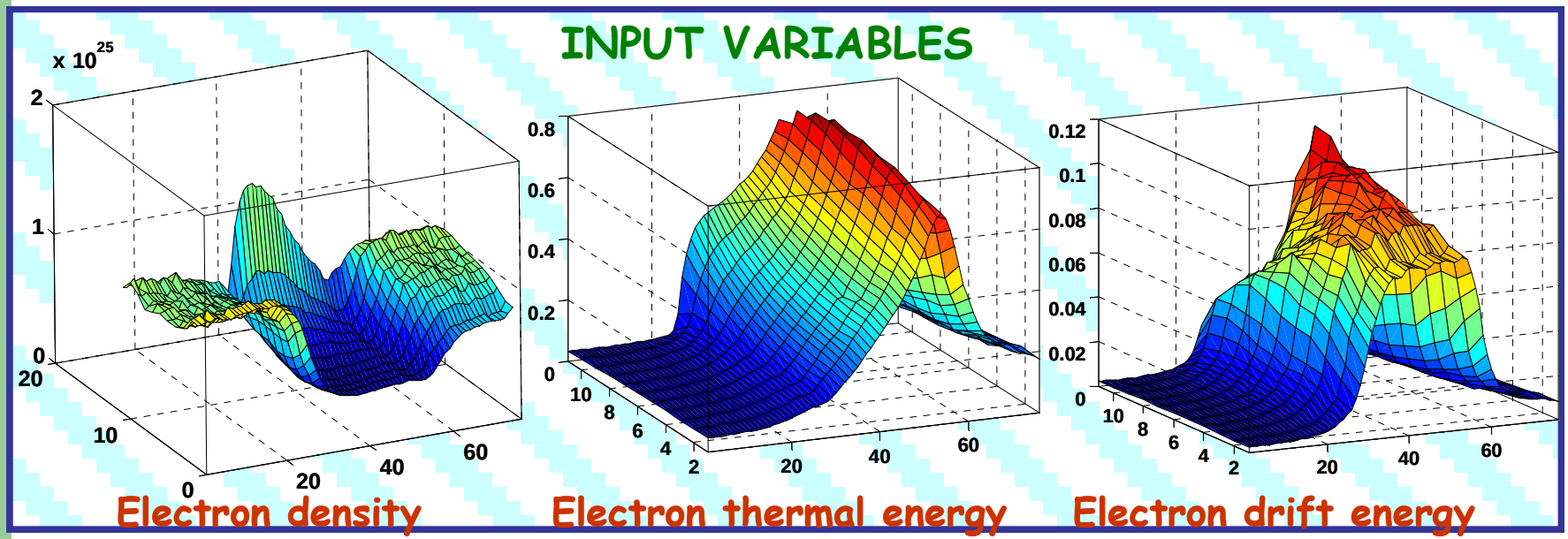
$$G_\phi(\mathbf{r},t) = 0$$

$$R_\phi(\mathbf{r},t) = -\left(\frac{\partial n}{\partial t}\right)_{coll}$$

- Using $\mathbf{v}=\mathbf{v}_d+\mathbf{c}$, one gets the final form of the balance equation for the carrier density:

$$\boxed{\frac{\partial n}{\partial t} = -\nabla\cdot(n\mathbf{v}_d) + \left(\frac{\partial n}{\partial t}\right)_{coll}}$$

Drift vs. Thermal Energy in FD SOI



Channel Length = 25 nm
Tsi = 10 nm

Momentum

- Momentum Balance equation is obtained by assuming that $\phi(\mathbf{p})=\mathbf{p}$:

$$\Phi(\mathbf{r},t) = \mathbf{P}_d = n\mathbf{p}_d$$

$$\mathbf{J}_\phi(\mathbf{r},t) = \mathbf{J}_\mathbf{p}(\mathbf{r},t) = \int d\mathbf{p}\mathbf{v}(\mathbf{p})\mathbf{p}f(\mathbf{r},\mathbf{p},t)$$

$$G_\phi(\mathbf{r},t) = -en\mathbf{E}$$

$$R_\phi(\mathbf{r},t) = -\left(\frac{\partial(n\mathbf{p}_d)}{\partial t}\right)_{coll}$$

- This leads to the following momentum balance equation:

$$\frac{\partial(n\mathbf{p}_d)}{\partial t} = -\nabla\cdot\mathbf{J}_\mathbf{p} - en\mathbf{E} + \left(\frac{\partial(n\mathbf{p}_d)}{\partial t}\right)_{coll}$$

Momentum, Cont'd

- For the flow of the momentum component p_x we have that:

$$\nabla \cdot \mathbf{J}_{p_x} = \nabla \cdot \int dp \mathbf{v} p_x f = \frac{\partial J_{p,xx}}{\partial x} + \frac{\partial J_{p,yx}}{\partial y} + \frac{\partial J_{p,zx}}{\partial z}$$

- Using again $\mathbf{v}=\mathbf{v}_d+\mathbf{c}$, one gets:

$$J_{p,ij} = \int d\mathbf{p} v_i p_j f = nm * v_{di} v_{dj} + nm * \left\langle c_i c_j \right\rangle$$

- Assuming diagonal temperature tensor, the above equation simplifies to:

$$\nabla \cdot \mathbf{J}_{p_x} = \frac{\partial (n v_{dx} p_{dx})}{\partial x} + \frac{\partial (n v_{dy} p_{dx})}{\partial y} + \frac{\partial (n v_{dz} p_{dx})}{\partial z} + \frac{\partial (n k_B T)}{\partial z}$$

- The <u>final form</u> of the momentum balance equation is:

$$\boxed{\frac{\partial (n\mathbf{p}_d)}{\partial t} = -\nabla \cdot (n\mathbf{v}_d \mathbf{p}_d) - \nabla (n k_B T) - en\mathbf{E} + \left(\frac{\partial (n\mathbf{p}_d)}{\partial t} \right)_{coll}}$$

Energy

- The Energy Balance equation is obtained by assuming that $\phi(\mathbf{p})=E(\mathbf{p})$:

$$\Phi(\mathbf{r},t) = W = nw$$

$$\mathbf{J}_\phi(\mathbf{r},t) = \mathbf{J}_W(\mathbf{r},t) = \int d\mathbf{p}\mathbf{v}(\mathbf{p})E(\mathbf{p})f(\mathbf{r},\mathbf{p},t)$$

$$= nw\mathbf{v}_d + nk_BT\mathbf{v}_d + n\mathbf{q}$$

$$G_\phi(\mathbf{r},t) = -e\mathbf{E}\cdot(n\mathbf{v}_d)$$

$$R_\phi(\mathbf{r},t) = -\left(\frac{\partial(nw)}{\partial t}\right)_{coll}$$

- The energy balance equation is then of the form:

$$\frac{\partial(nw)}{\partial t} = -\nabla\cdot(nw\mathbf{v}_d + nk_BT\mathbf{v}_d + n\mathbf{q}) - en\mathbf{E}\cdot\mathbf{v}_d + \left(\frac{\partial(nw)}{\partial t}\right)_{coll}$$

Closure

- To have a closed set of equations, one either:
  (a) ignores the heat flux altogether
  (b) uses a simple recipe for the calculation of the heat flux:

$$n\mathbf{q} = -\kappa \nabla T, \qquad \kappa = \frac{5k_B^2 nT}{2m^* v(w)}$$

- Substituting T with the density of the carrier energy, the momentum and energy balance equations become:

$$\frac{\partial(n\mathbf{p}_d)}{\partial t} = -\nabla \cdot (n\mathbf{v}_d \mathbf{p}_d) - \frac{2}{3}\nabla\left(nw - \frac{1}{2}nm^* v_d^2\right) - en\mathbf{E} + \left(\frac{\partial(n\mathbf{p}_d)}{\partial t}\right)_{coll}$$

$$\frac{\partial(nw)}{\partial t} = -\nabla \cdot \left[n\mathbf{v}_d w + \frac{2}{3}\nabla\left(n\mathbf{v}_d - \frac{\kappa}{k_B}\nabla\right)\left(w - \frac{1}{2}m^* v_d^2\right)\right]$$

$$- en\mathbf{E} \cdot \mathbf{v}_d + \left(\frac{\partial(nw)}{\partial t}\right)_{coll}$$

Balance Equations

- More convenient set of balance equations is in terms of n, $\boldsymbol{v}_d$ and w:

$$\frac{\partial(n)}{\partial t} = -\nabla \cdot (n\mathbf{v}_d) + \left(\frac{\partial n}{\partial t}\right)_{coll}$$

$$\frac{\partial(\mathbf{v}_d)}{\partial t} = -\frac{\mathbf{v}_d}{m^*} \cdot \nabla(m^* \mathbf{v}_d) - \frac{2}{3nm^*}\nabla\left(nw - \frac{1}{2}nm^* v_d^2\right) - \frac{e\mathbf{E}}{m^*} + \left(\frac{\partial(\mathbf{v}_d)}{\partial t}\right)_{coll}$$

$$\frac{\partial(w)}{\partial t} = -\mathbf{v}_d \cdot \nabla w - \frac{2}{3n}\nabla \cdot \left[\left(n\mathbf{v}_d - \frac{\kappa}{k_B}\nabla\right)\left(w - \frac{m^* v_d^2}{2}\right)\right] - e\mathbf{E} \cdot \mathbf{v}_d + \left(\frac{\partial(w)}{\partial t}\right)_{coll}$$

Reduction to Drift-Diffusion Model

- The DD model is obtained by simplifying the momentum balance equation, which in 1D is of the form:

$$\frac{\partial(P_{dz})}{\partial t} = -\frac{\partial}{\partial z}(nv_d p_d) - \frac{\partial}{\partial z}(nk_B T) - enE + \left(\frac{\partial(P_z)}{\partial t}\right)_{coll}$$
$$= -\frac{\partial}{\partial z}(2nw) - enE - \left\langle \frac{1}{\tau_m} \right\rangle P_z$$

- In steady-state, one gets for the momentum balance equation that:

$$J_z = ne\mu_n[E + E'] + eD_n \frac{\partial n}{\partial z} \qquad \text{where:} \qquad E' = \frac{2}{e}\frac{\partial w}{\partial z}$$
$$D_n = \frac{2\mu_n w}{e}$$

Simplifications

- The DD model is then obtained by making the following assumptions:
  - The distribution function is close to the equilibrium value
  - The energy gradient field is zero.
  - In the extended DD model $\mu(E)$ and $D(E)$ are assumed to depend upon the local field values only.

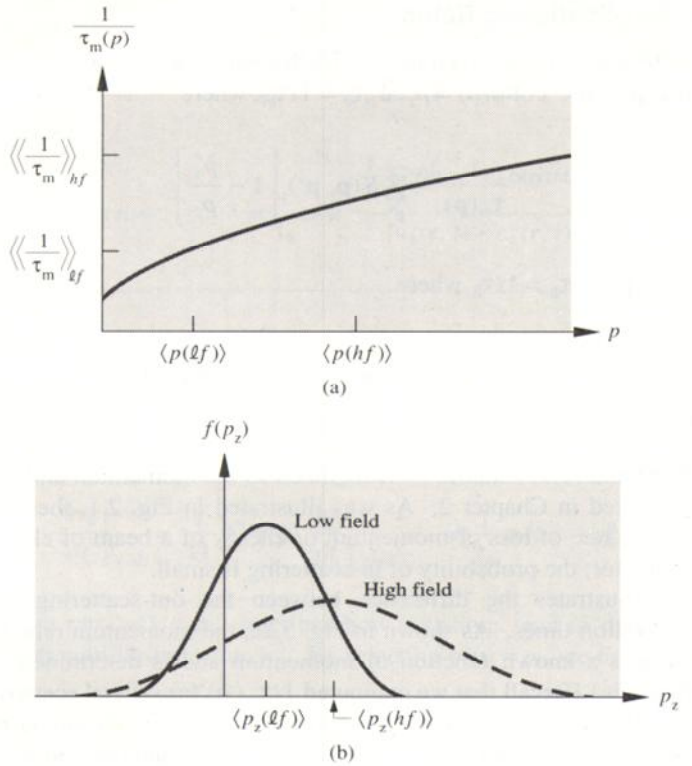
Ensemble Relaxation Rates

- To see how one can calculate the momentum and the energy ensemble relaxation rates, it is necessary to go back to the definition of R_ϕ:

$$R_\phi = \nu_\phi(\Phi - \Phi_0)$$
$$= -\int d\mathbf{p}\phi(\mathbf{p})\frac{\partial f}{\partial t}\bigg|_{coll}$$
$$= \int d\mathbf{p}\,\frac{\phi(\mathbf{p})f(\mathbf{r},\mathbf{p},t)}{\tau_\phi(\mathbf{p})}$$

where the relaxation time τ_ϕ is:

$$\frac{1}{\tau_\phi(\mathbf{p})} = \sum_{\mathbf{p}'}\left[1-\frac{\phi(\mathbf{p}')}{\phi(\mathbf{p})}\right]S(\mathbf{p},\mathbf{p}')$$

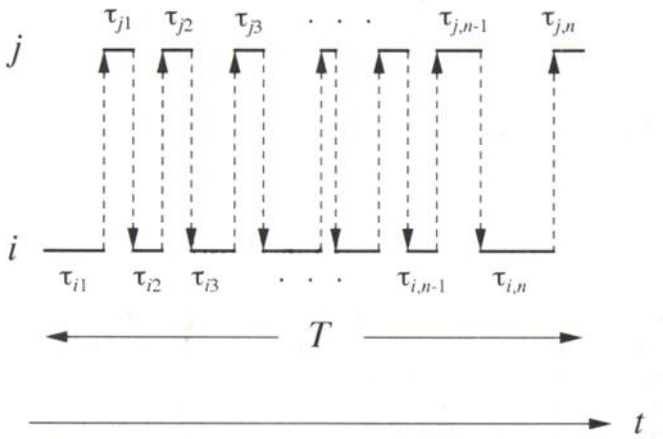


Ensemble Relaxation Rates

- The ensemble relaxation rate, which appears in the carrier density balance equation, is related to the intervalley transfer in many-valley semiconductors. It equals to:

$$\left(\frac{\partial n}{\partial t}\right)_{coll} = -\nu_n (n - n_0)$$

One usually calculates this ensemble relaxation rate by using Monte Carlo simulation:



$$\nu_{n,ij} = \frac{N_{i\to j}}{T_i}$$

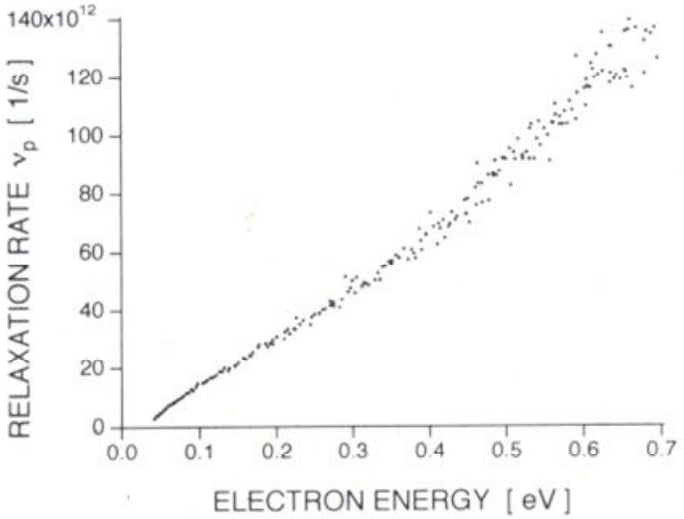
$$\nu_{n,ji} = \frac{N_{j\to i}}{T_j}$$

Momentum Relaxation Rate

- The momentum rate is determined by a steady-state MC calculation in a bulk semiconductor under a uniform bias electric field, for which:

$$\frac{\partial \mathbf{v}_d}{\partial t} = -\frac{e\mathbf{E}}{m^*} + \left(\frac{\partial \mathbf{v}_d}{\partial t}\right)_{coll} = -\frac{e\mathbf{E}}{m^*} - \nu_p(w)\mathbf{v}_d = 0$$

$$\nu_p(w) = \frac{eE}{m^* v_d}$$

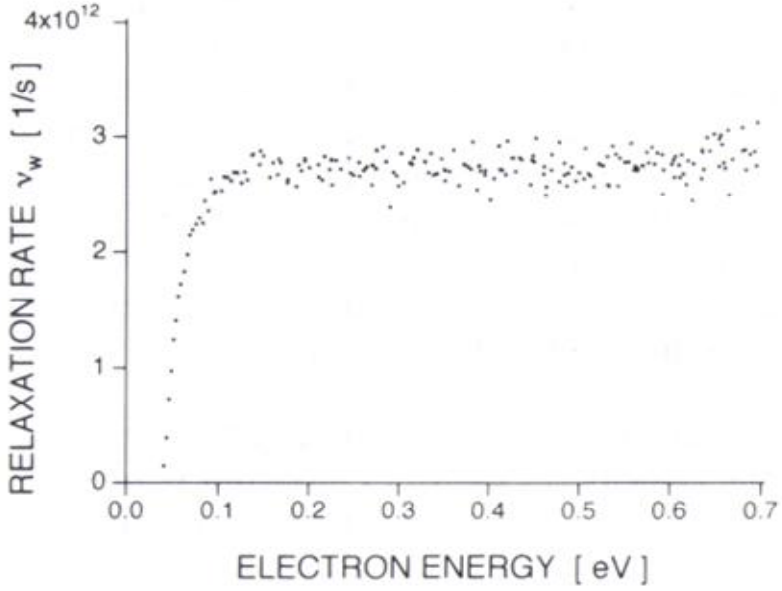


Energy Relaxation Rate

- The emsemble energy relaxation rate is also determined by a steady-state MC calculation in a bulk semiconductor under a uniform bias electric field, for which:

$$\frac{\partial w}{\partial t} = -e\mathbf{E}\cdot\mathbf{v}_d + \left(\frac{\partial w}{\partial t}\right)_{coll} = -e\mathbf{E}\cdot\mathbf{v}_d - \nu_w(w - w_0) = 0$$

$$\nu_w(w) = -\frac{e\mathbf{E}\cdot\mathbf{v}_d}{w - w_0}$$



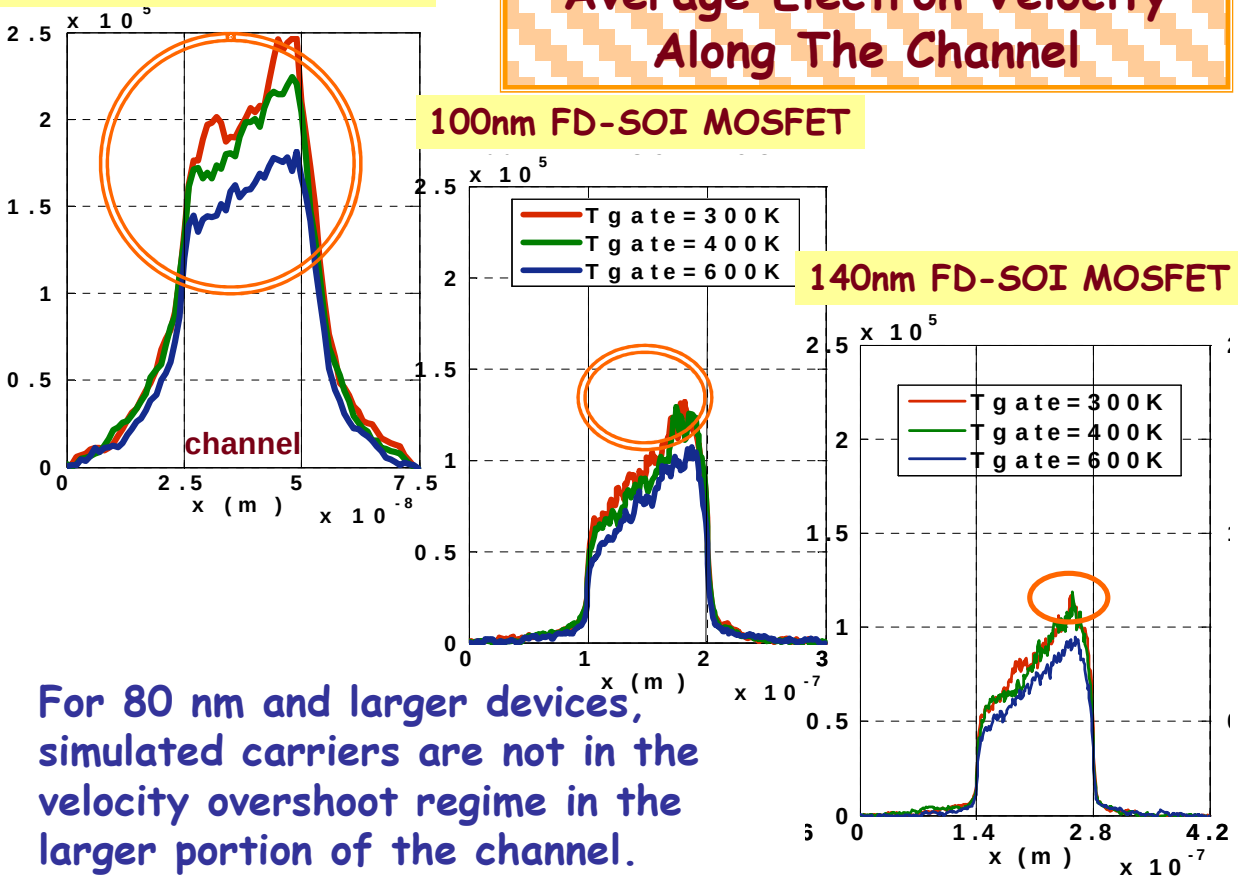
Simulation Example – Importance of Velocity Overshoot

25nm FD-SOI MOSFET

Average Electron Velocity Along The Channel

100nm FD-SOI MOSFET

140nm FD-SOI MOSFET



For 80 nm and larger devices, simulated carriers are not in the velocity overshoot regime in the larger portion of the channel.

Discretization of the Balance Equations

- For simplicity, the equations will be discretized on an equally spaced meshes. In 1D and in finite-difference operator notation, the RHS's of the equations that need to be solved are:

$$G_{n,i} = -n_i L_x(v_i) - v_i L_x(n_i)$$

$$G_{v,i} = -v_i L_x(v_i) - \frac{2}{3n_i m^*} L_x\left(n_i w_i - \frac{1}{2} n_i m^* v_i^2\right) - \frac{eE_i}{m^*} - \nu_p(w_i) v_i$$

$$G_{w,i} = -v_i L_x(w_i) - \frac{2}{3n_i} L_x\left[n_i v_i \left(w_i - \frac{m^* v_i^2}{2}\right)\right]$$

$$+ \frac{2\kappa}{3n_i k_B} L_{xx}\left(w_i - \frac{m^* v_i^2}{2}\right) - eE_i v_i - \nu_w(w_i)(w_i - w_0)$$

$$G_{\varphi,i} = L_{xx}(\varphi_i) + \frac{e}{\varepsilon}(N_{D,i} - n_i)$$

Discretization of the Balance Equations (Cont'd)

- The various explicit schemes that one can use are listed below:

(a) Forward-time centered-space scheme (FTCS):

$$L_x[f_i] = \frac{f_{i+1} - f_{i-1}}{2\Delta x}, \qquad L_{xx}[f_i] = \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2}, \qquad \left.\frac{\partial f}{\partial t}\right|_i \approx \frac{f_i^f - f_i}{\Delta t}$$

(b) Upwind scheme:

$$v_i L_x^{uw}[f_i] = \begin{cases} v_i \dfrac{f_i - f_{i-1}}{\Delta x}, & v_i \geq 0 \\ v_i \dfrac{f_{i+1} - f_i}{\Delta x}, & v_i < 0 \end{cases}$$

(c) Lax-Wendroff scheme:

$$v_i L_x^{LW}[f_i] = v_i L_x[f_i] - v_i^2 \frac{\Delta t}{2} L_{xx}[f_i]$$

Discretization of the Balance Equations (cont'd)

(d) DuFort-Frankel scheme:

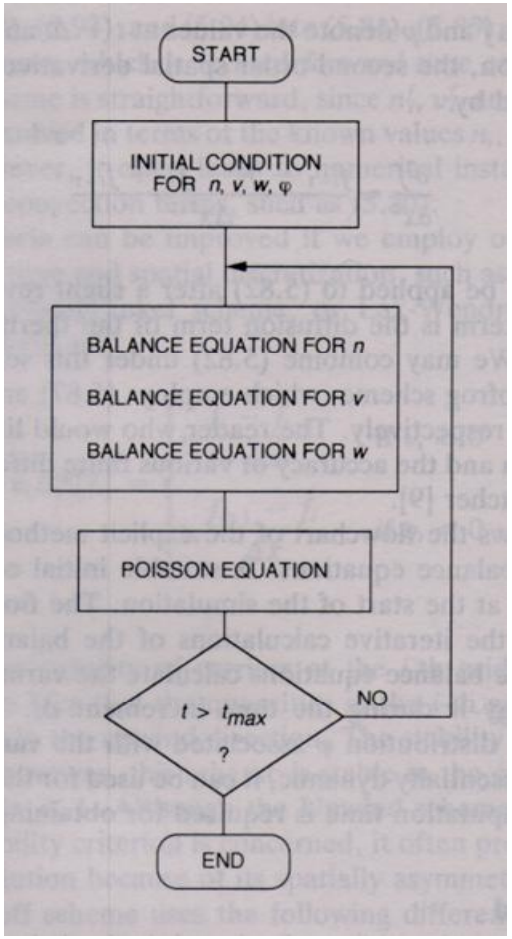
$$L_{xx}[f_i] = \frac{f_{i-1} - f_i^f - f_i^p + f_{i+1}}{\Delta x^2}$$

$$\left.\frac{\partial f}{\partial t}\right|_i \approx \frac{f_i^f - f_i^p}{2\Delta t}$$

(e) Leapfrog scheme:

$$L_x^{lf}[f_i] = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

$$\left.\frac{\partial f}{\partial t}\right|_i \approx \frac{f_i^f - f_i^p}{2\Delta t}$$



Energy Balance Model Implementation in Silvaco

For a detailed description of the energy balance/hydrodynamic model please review the lecture notes on hydrodynamic modeling.

Important features of this example are:

- The **MATERIAL** statement is used to assign the energy relaxation times **(taurel.el, taumob.el, …)**
- The **MODELS** statement is used to select the physical models used **(hcte)**
- The **IMPACT** statement is used to assign the energy relaxation length for the Selberherr model

Only parts of the listing that are relevant for the device simulation part are extracted in the next few slides.

More Details

E.TAUR.VAR specifies that electron temperature dependent energy relaxation time is used. Use parameters TRE.T1, TRE.T2, TRE.T3, TRE.W1, TRE.W2 and TRE.W3 on material statement to specifie the energy relaxation time.

H.TAUR.VAR specifies that hole temperature dependent energy relaxation time is used. Use parameters TRH.T1, TRH.T2, TRH.T3, TRH.W1, TRH.W2 and TRH.W3 on material statement to specifie the energy relaxation time.

HCTE specifies that both electron and hole temperature will be solved.

HCTE.**EL** specifies that electron temperature will be solved.

HCTE.**HO** specifies that hole temperature will be solved.

F.KSN specifies the name of a file containing a C interpreter function specifying the electron Peltier coefficient as a function of electron energy.

F.KSP specifies the name of a file containing a C interpreter function specifying the hole Peltier coefficient as a function of hole energy.

KSN specifies which hot carrier transport model will be used for electrons. KSN=0 selects the hydrodynamic model and KSN=-1 selects the energy balance model.

KSP specifies which hot carrier transport model will be used for holes. KSP=0 selects the hydrodynamic model and KSP=-1 selects the energy balance model.

More Details …

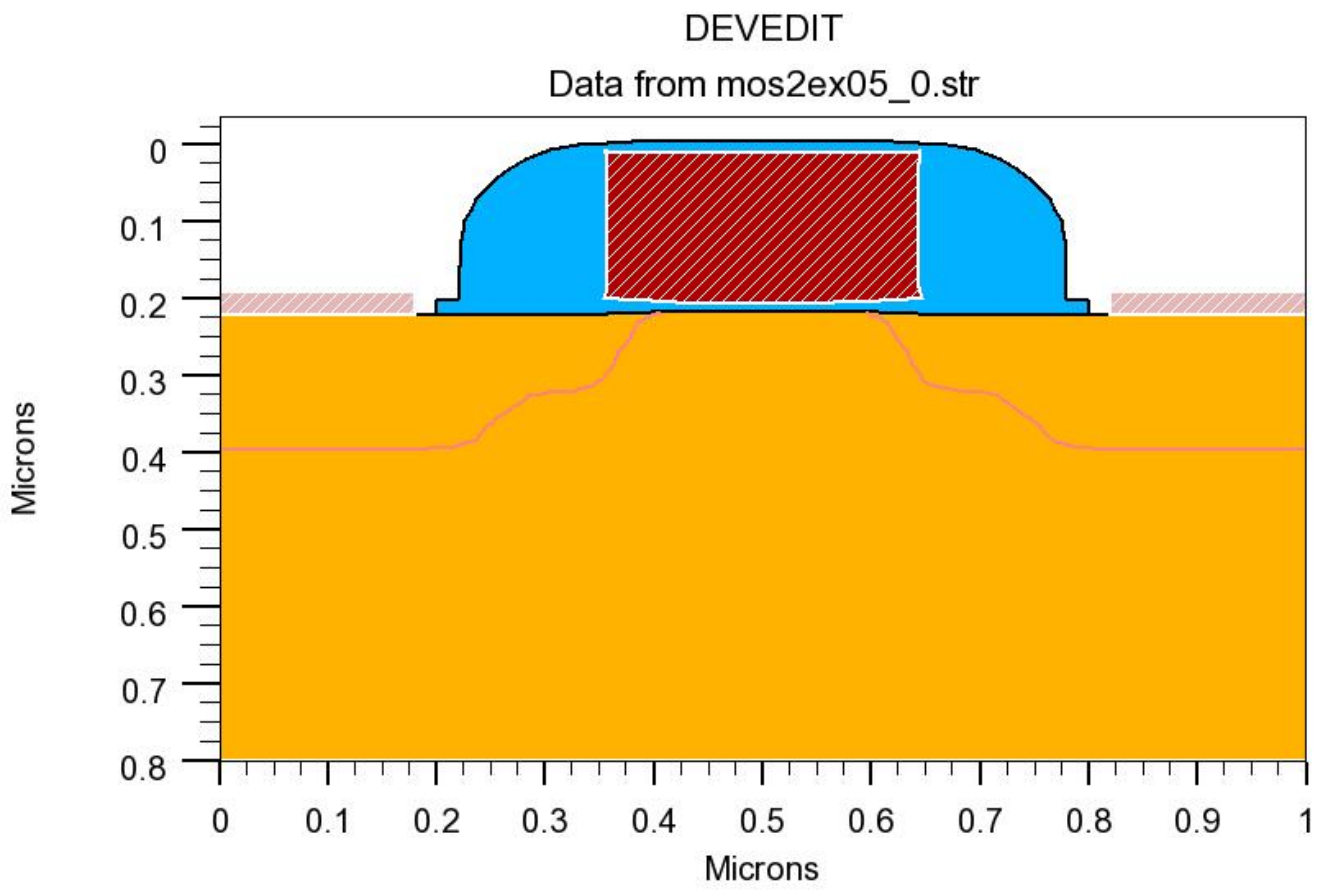
TAUMOB specifies the dependence of relaxation times with carrier temperature in the mobility definition. If TAUMOB is specified, the values of MATERIAL statement parameters TAUMOB.EL and TAUMOB.HO are dependent on the carrier temperature.

TAUTEM specifies the dependence of relaxation times with carrier temperature. If TAUTEM is specified, the values of MATERIAL statement parameters TAUREL.EL and TAUREL.HO are dependent on carrier temperature..

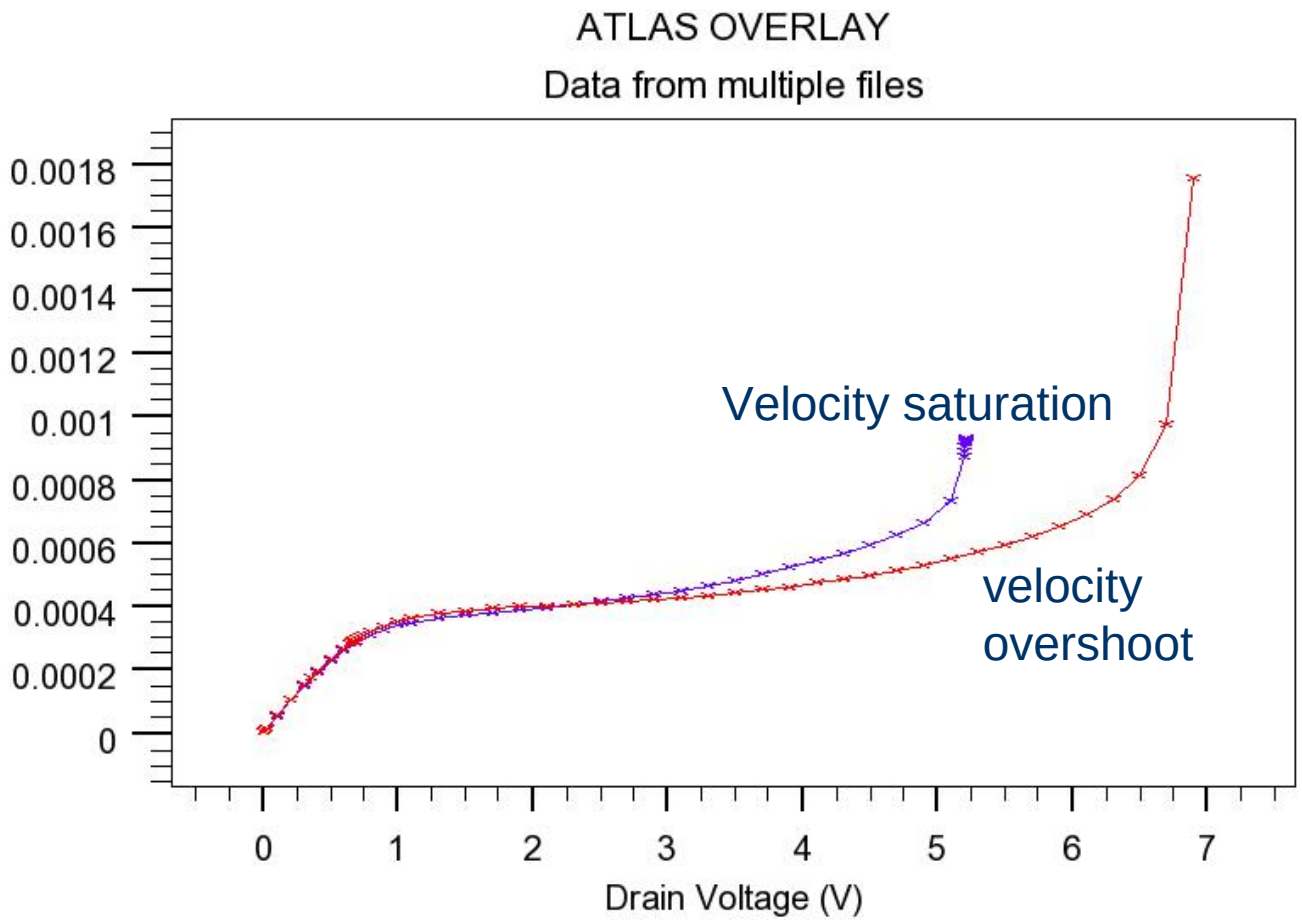
N.**TEMP** or **HCTE.EL** specifies that the electron temperature equation will be solved.

P.**TEMP** or **HCTE.HO** specifies that the hole temperature equation will be solved.

Structure Being Simulated



Simulation results: DD vs. Energy Balance

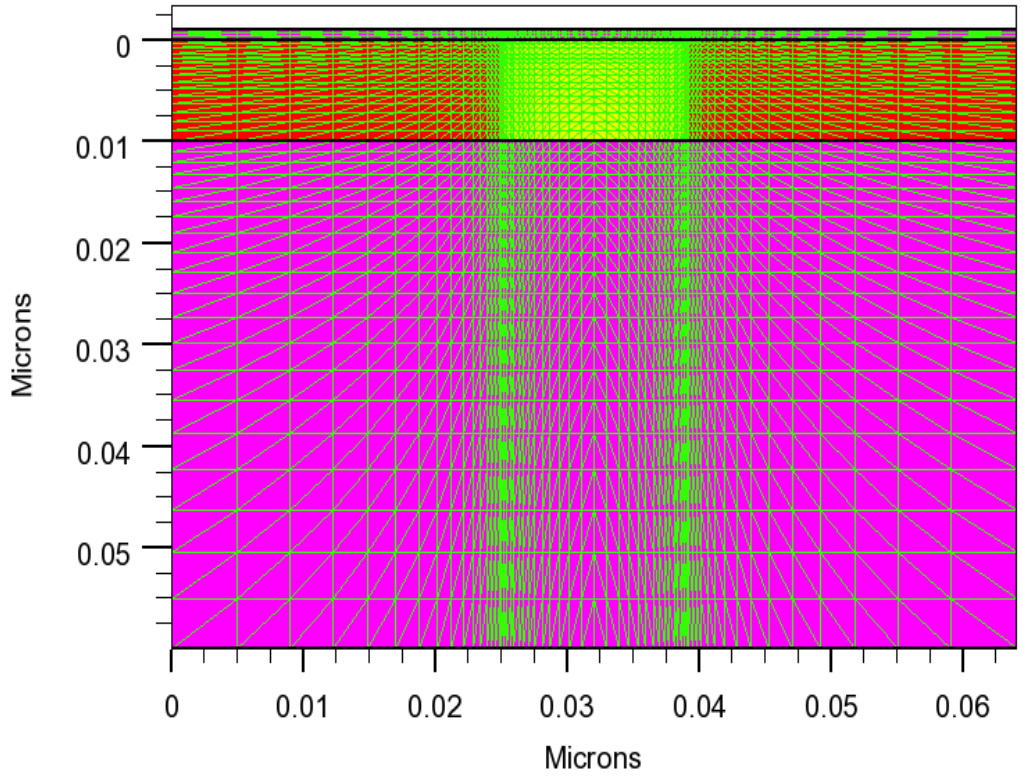


FD Device Generations Examined

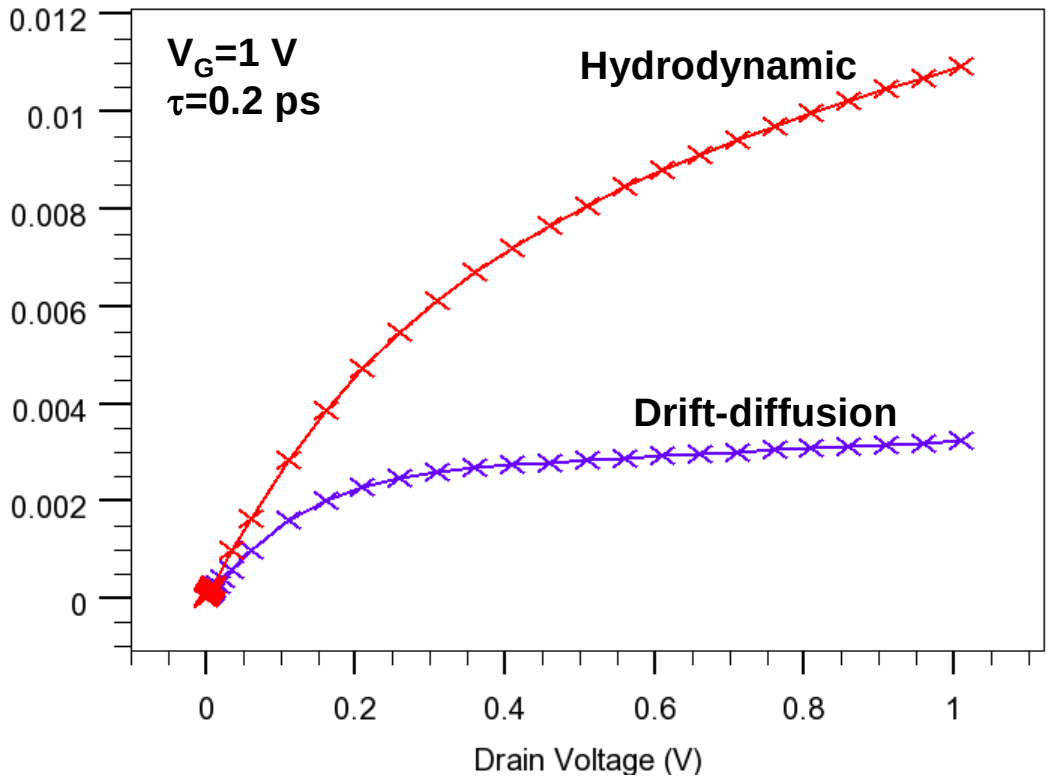
feature	14 nm	25 nm	90 nm
Tox	1 nm	1.2 nm	1.5 nm
VDD	1V	1.2 V	1.4 V

Source/drain doping = 10^{20} cm^{-3}
Channel doping = 10^{18} cm^{-3}

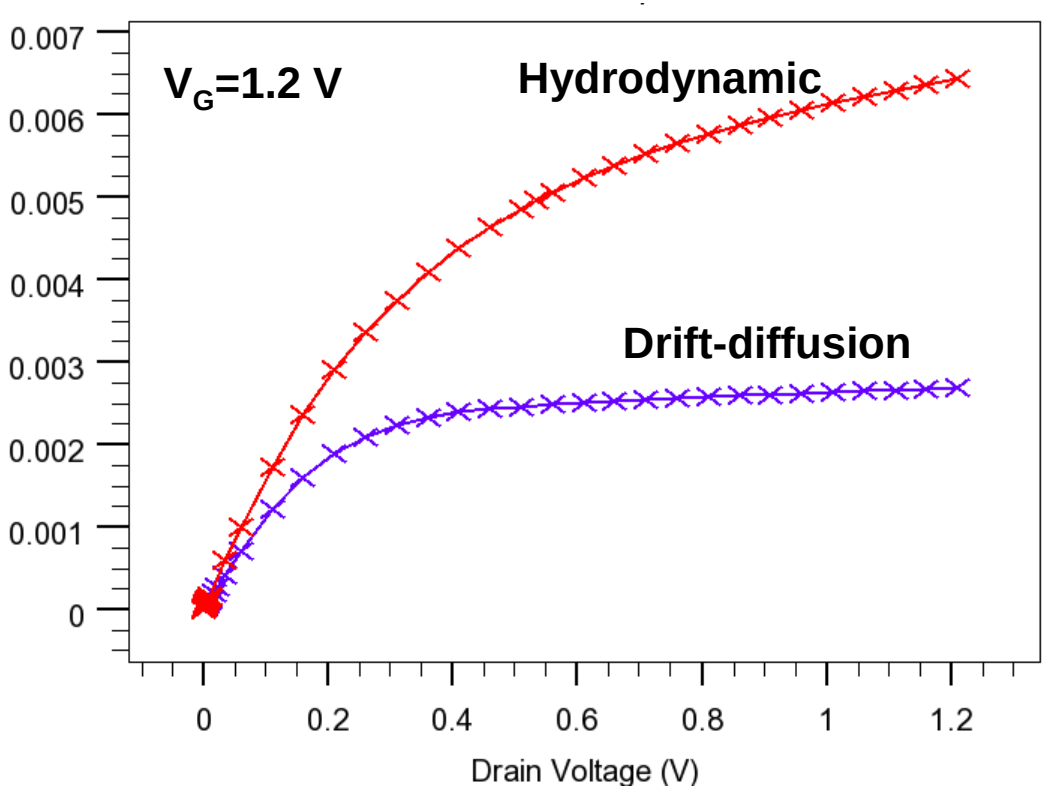
What happens in a 14 nm FD SOI Device?



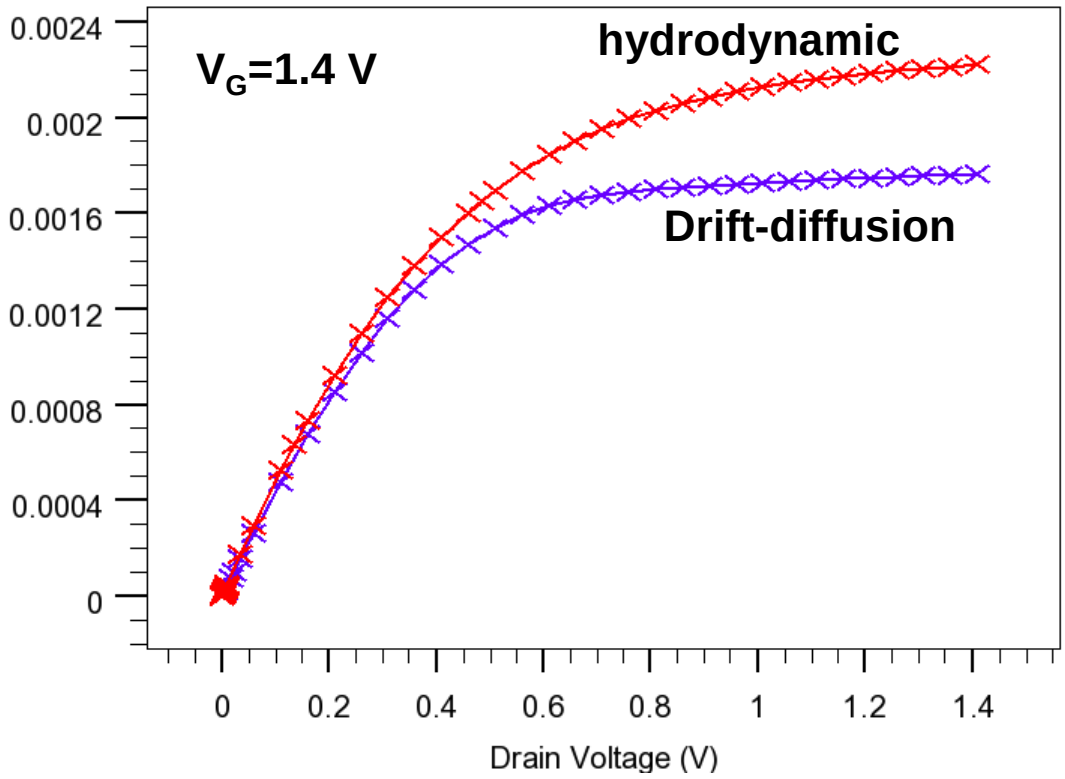
Results for 14 nm FD SOI Device



Results for 25 nm FD SOI Device



Results for 90 nm FD SOI Device



Results from Hydrodynamic Simulations

Device Structures Being Simulated

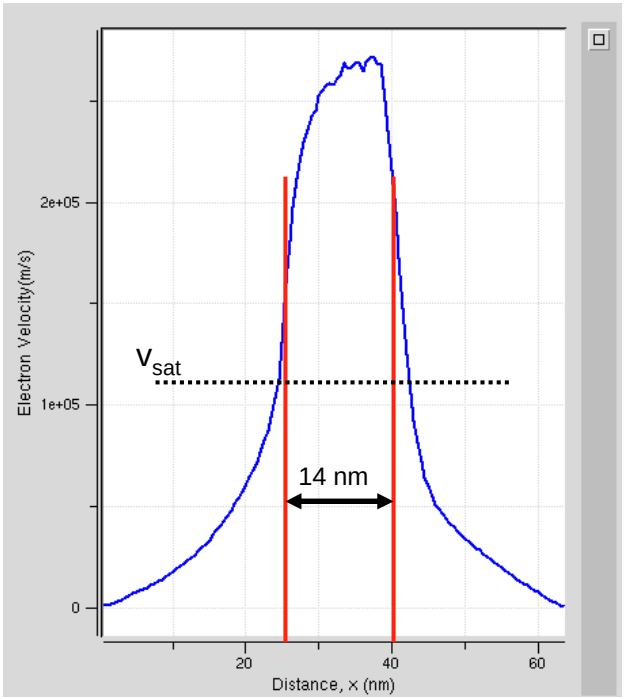
feature	14 nm	25 nm	90 nm
Tox	1 nm	1.2 nm	1.5 nm
VDD	1V	1.2 V	1.4 V
overshoot	240%	136%	22%

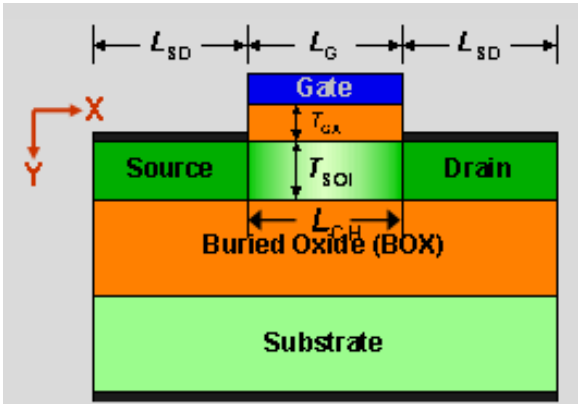
Source/drain doping = 1E20 cm^{-3}
Channel doping = 1E18 cm^{-3}

Overshoot= $(ID_{HD}-ID_{DD})/ID_{DD}$ (%) at on-state

Hydrodynamic Simulations

- In summary, we need to use at least hydrodynamic model to describe the velocity overshoot in nanoscale devices





We have non-stationary transport throughout the whole channel length (almost ballistic transport)

Problems with Hydrodynamic Simulations