

Lecture 4

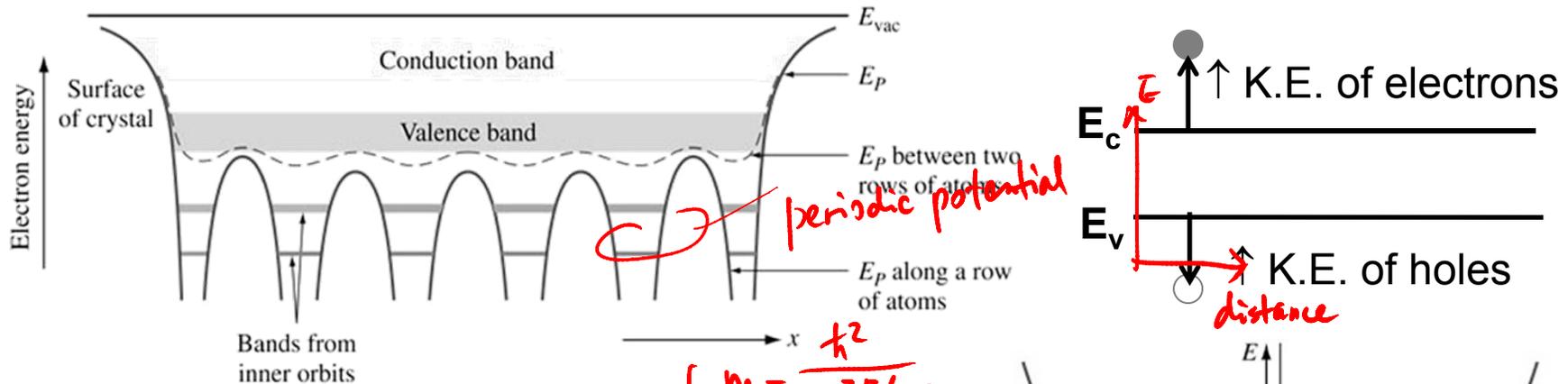
- MOSFET Transport Issues
 - semiconductor band structure
 - quantum confinement effects
 - low-field mobility and high-field saturation

Reading:

- M. Lundstrom, "[Fundamentals of Carrier Transport](#)," 2nd edition, *Cambridge University Press*, 2000.
- multiple research articles (reference list at the end of this lecture)

Dispersion Relationship: E vs. k

- E vs. distance in semiconductors

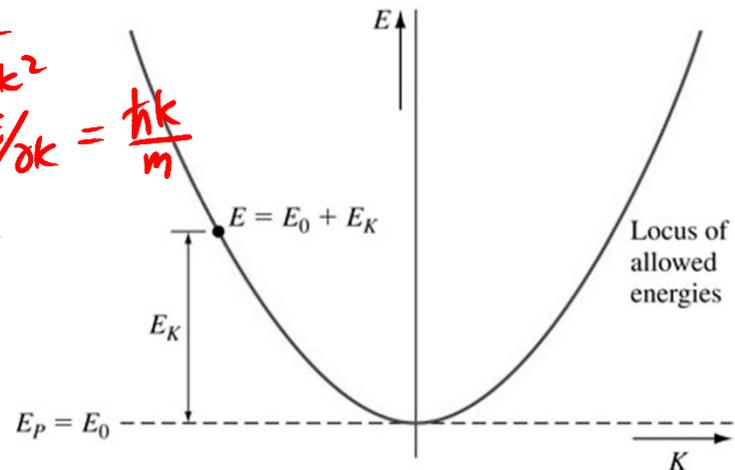


- Schrödinger equation

$$\frac{\hbar^2}{2m_0} \nabla^2 \psi + V(\mathbf{r})\psi = E\psi$$

$\psi \sim e^{i\mathbf{k}\cdot\mathbf{r}}$ called the plane wave solution
 $\mathbf{k} = \mathbf{k}_x + \mathbf{k}_y + \mathbf{k}_z$
 k is called the wave vector

$m = \frac{\hbar^2}{\partial^2 E / \partial k^2}$
 $v = \frac{1}{\hbar} \partial E / \partial k = \frac{\hbar k}{m}$
 $p = \hbar k$



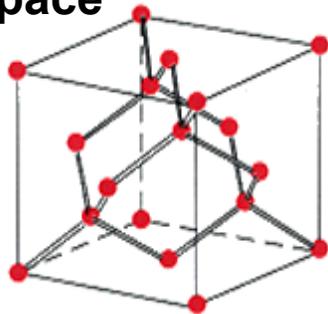
$$E = E_0 + \frac{\hbar^2 k^2}{2m}$$

If $V(\mathbf{r}) = 0$ (free electron): $m \rightarrow m_0$
 If $V(\mathbf{r}) = U(\vec{\mathbf{r}})$ (electron in crystal): $m \rightarrow m^*$

Semiconductor Band Structure

- Reciprocal space

Zinc-blende structure



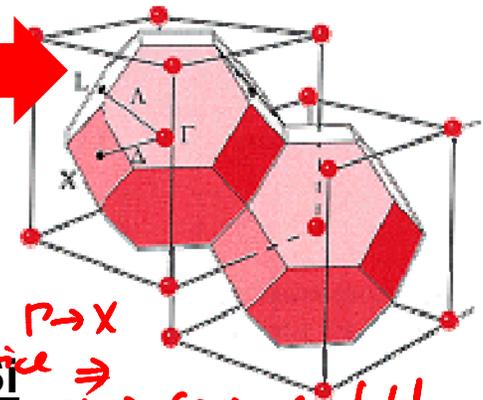
GaAs



[100] direction : $\Gamma \xrightarrow{\Delta} X$

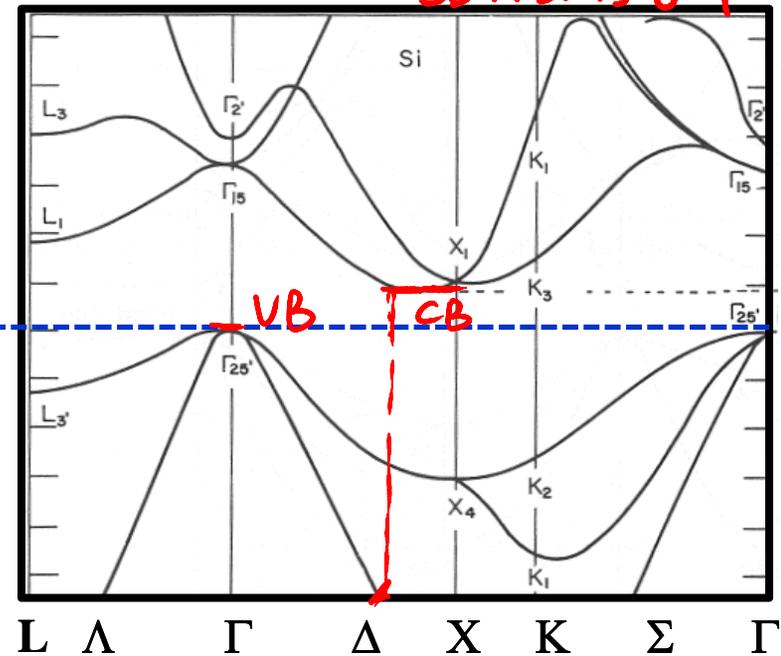
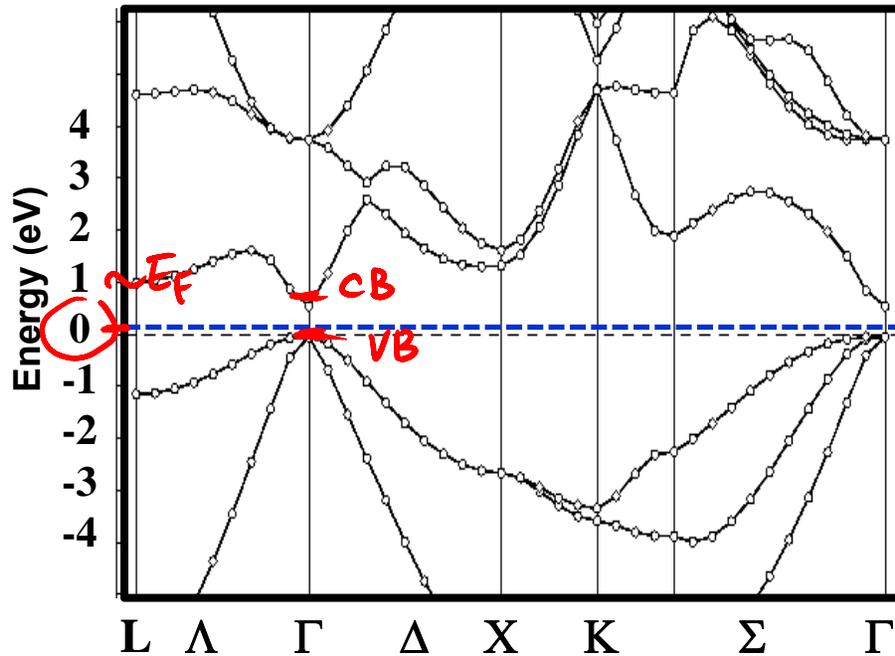
[111] direction : $\Gamma \xrightarrow{\Lambda} L$

[110] direction : $\Gamma \xrightarrow{\Sigma} K$



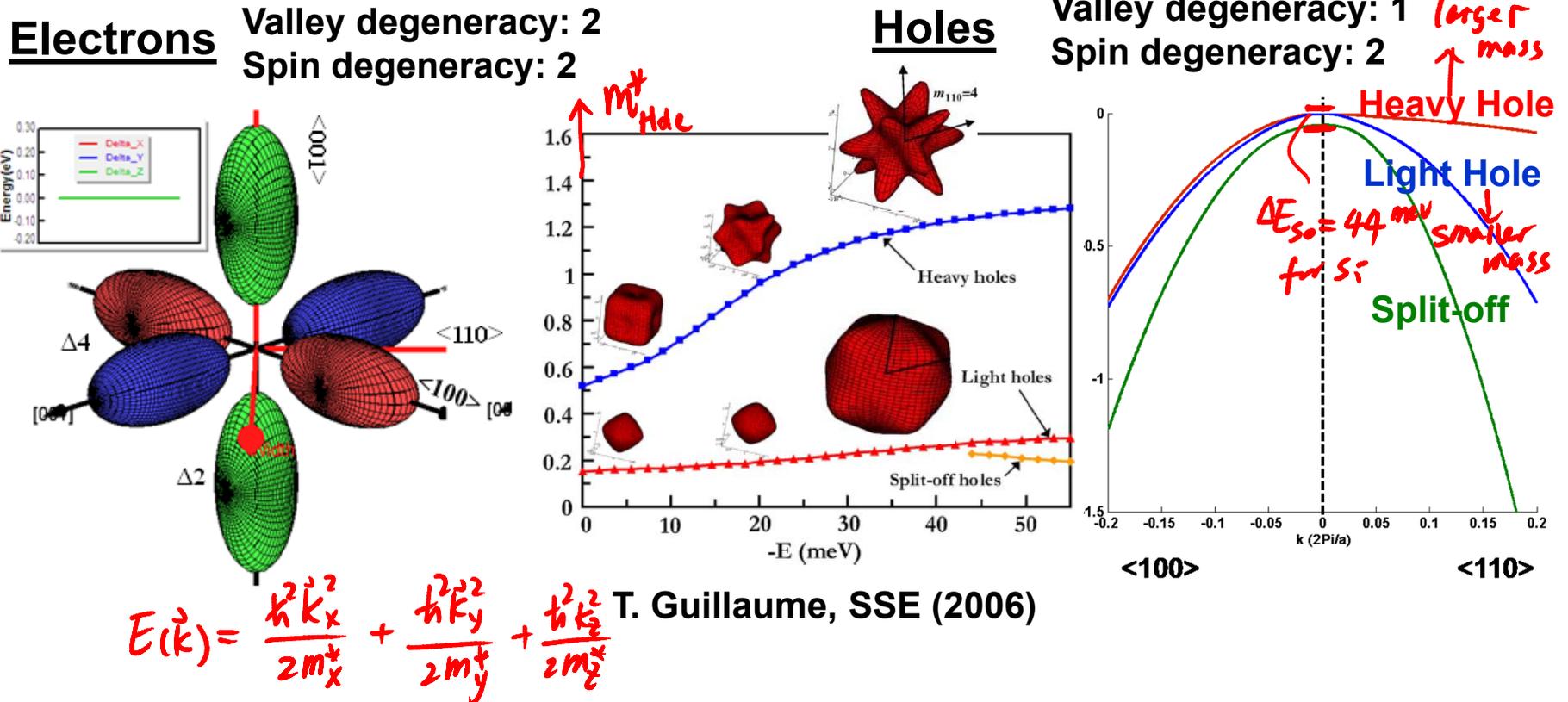
- E vs. k

there are totally 6 equivalent $\Gamma \rightarrow X$ in cubic lattice \Rightarrow CB in Si is 6-fold



Silicon Band Structure

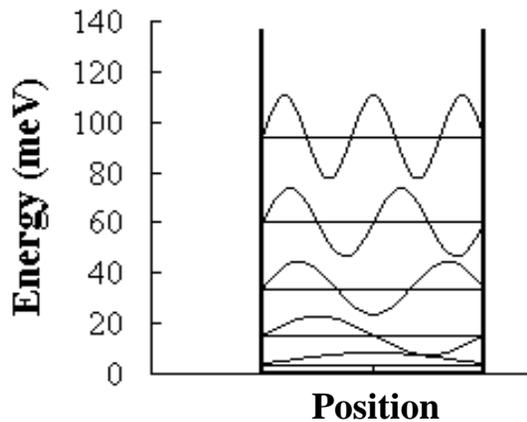
- Equi-energy contours



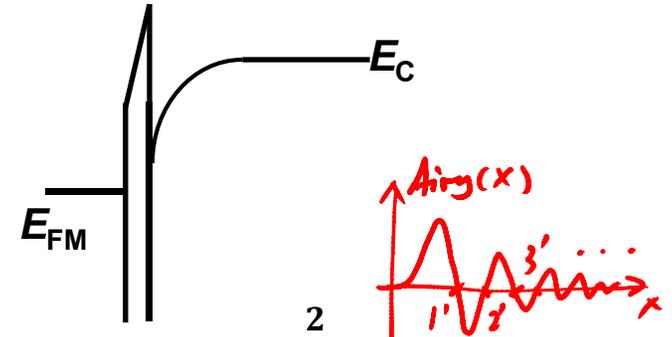
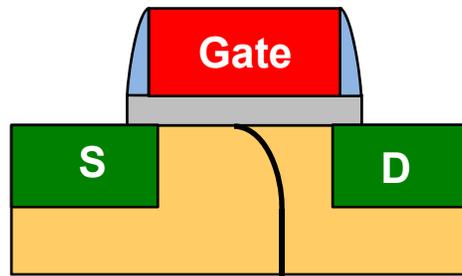
- E - k relationship is direction-dependent for electrons in solids.
- In Si, electrons have a more parabolic E - k relationship than holes.

Quantum Confinement (QC) Effects

- Sub-bands



In a MOS Inversion Layer:



Sub-band top/valley energies due to QC: $E_i = \left(\frac{3\pi q \hbar}{2\sqrt{2}m^*} F_s \right)^{2/3} \cdot \text{AiryRoots}(i)$

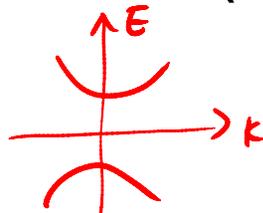
F. Stern, PRB (1972)

$dk \propto E^{-1/2} dE$ surface \vec{E} -field (S_i/S_iO_2)

- Reduced density-of-states (DOS)

3D Bulk:

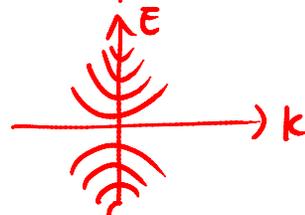
$$DOS(E) \equiv \frac{\# \text{ of } k \text{ states in } \Delta E}{\Delta E \cdot 3D \text{ Volume}}$$



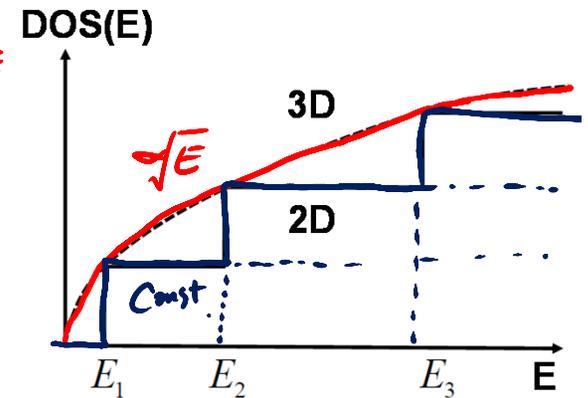
$DOS \propto \frac{\int dk^3}{dE} \propto \int E^{1/2} dE$

2D Inversion Layer:

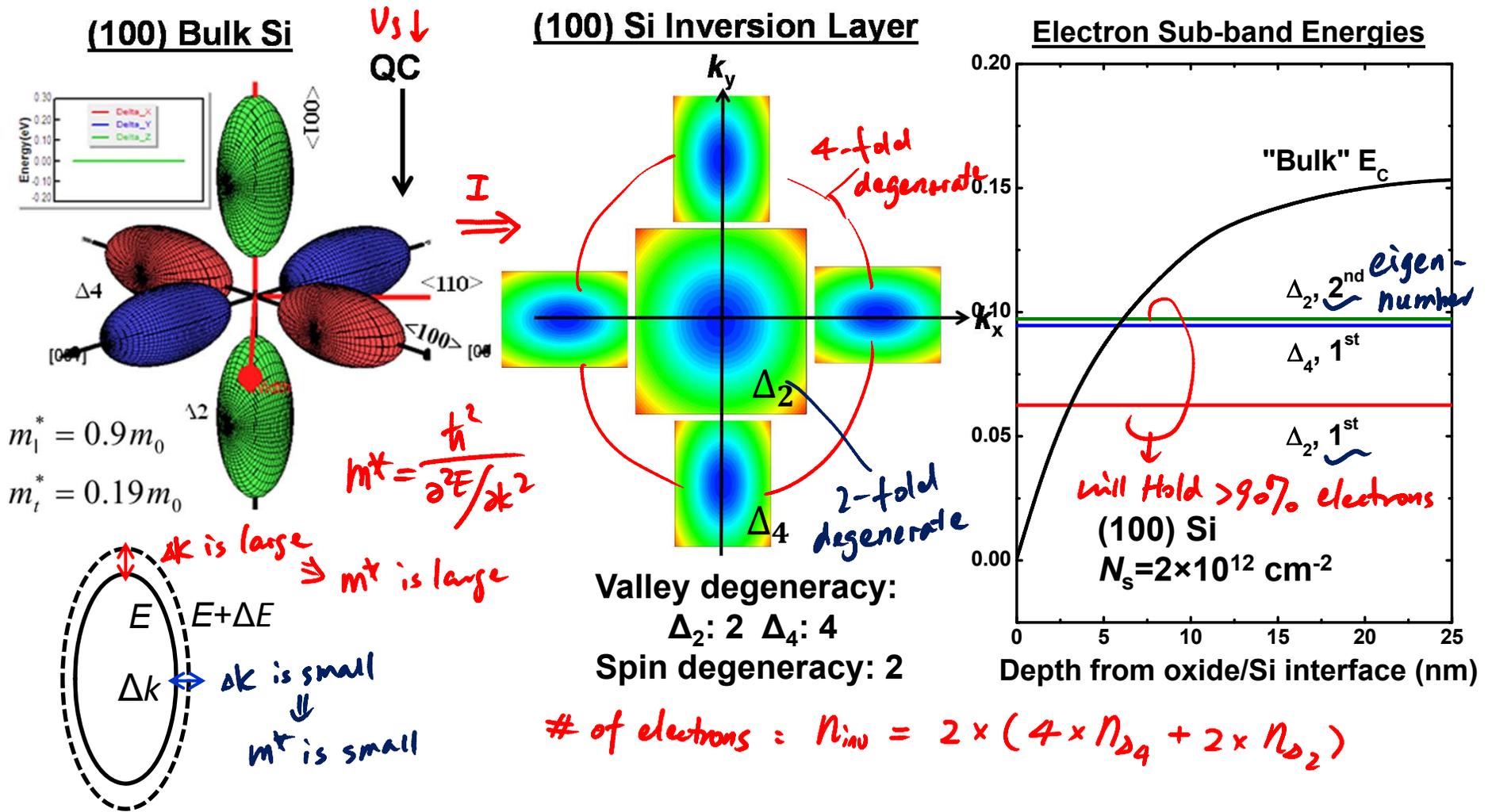
$$DOS(E) \equiv \frac{\# \text{ of } k \text{ states in } \Delta E}{\Delta E \cdot 2D \text{ Area}}$$



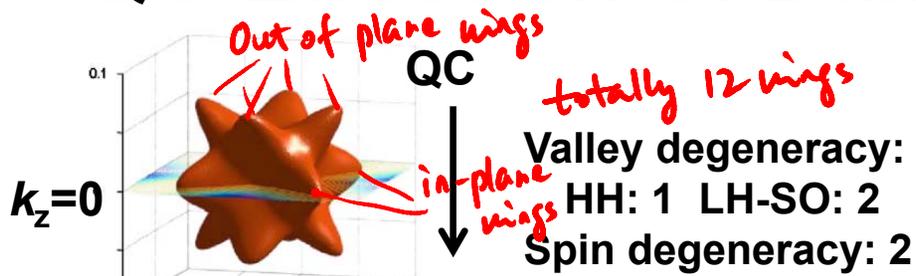
$DOS \propto \frac{\int dk^2}{dE} \propto \frac{\int dE}{const.}$



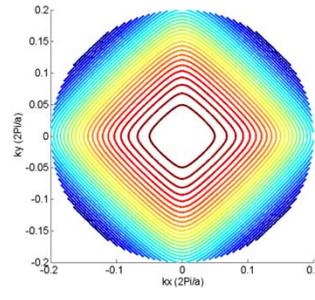
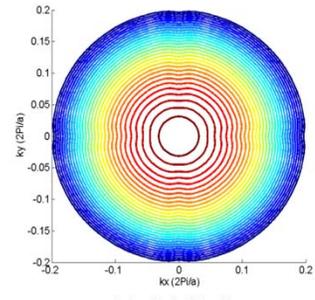
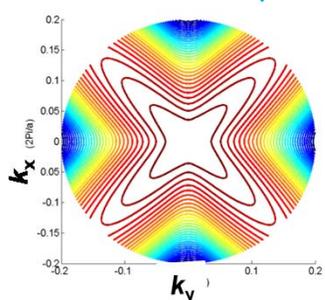
QC Effect on Si Band Structure: Electrons



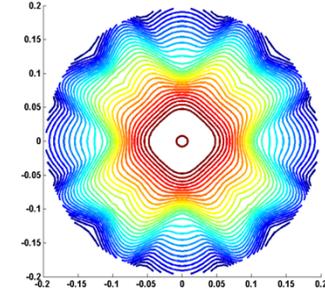
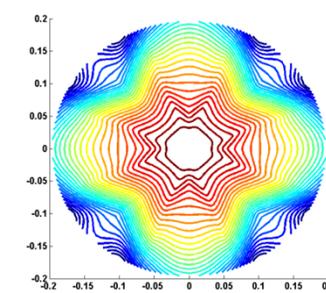
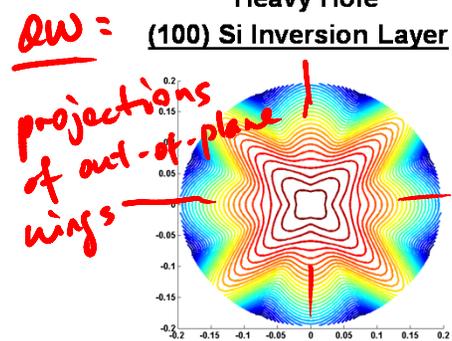
QC Effect on Si Band Structure: Holes



(100) Bulk Si

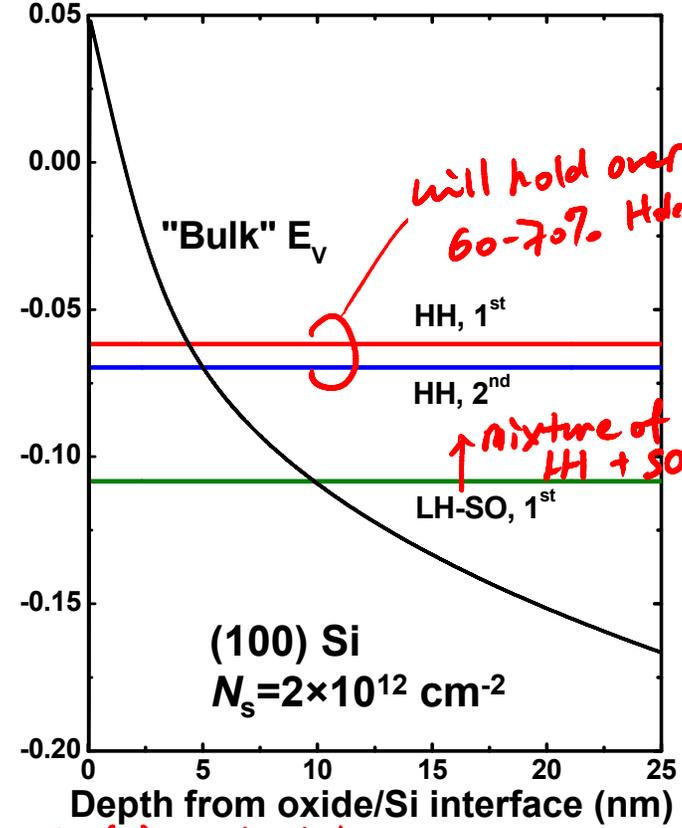


(100) Si Inversion Layer



N. Xu, Ph.D. thesis (2012)

Hole Sub-band Energies

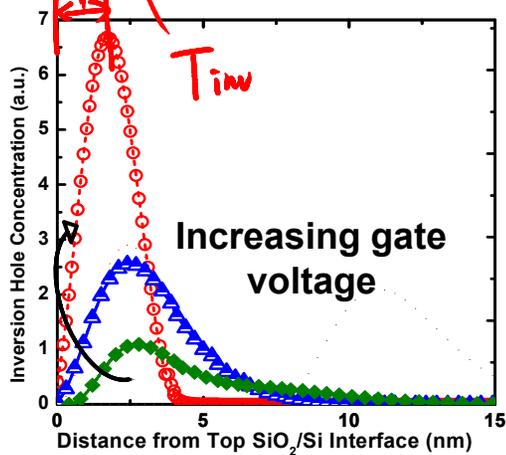


of inversion holes:

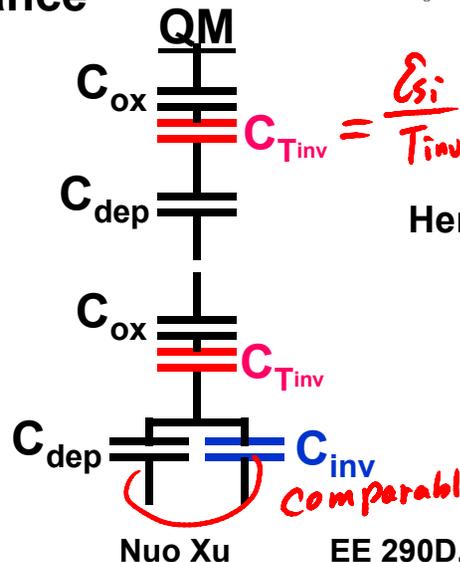
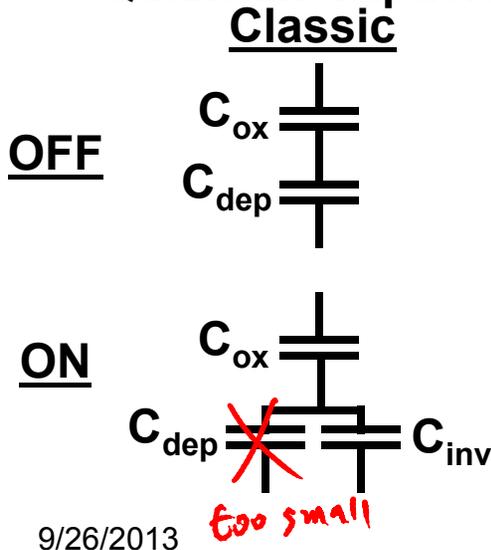
$$P_{inv} = (P_{HH} + P_{LH} + P_{SO}) \times 2$$

Impacts of QC on MOS Electrostatics

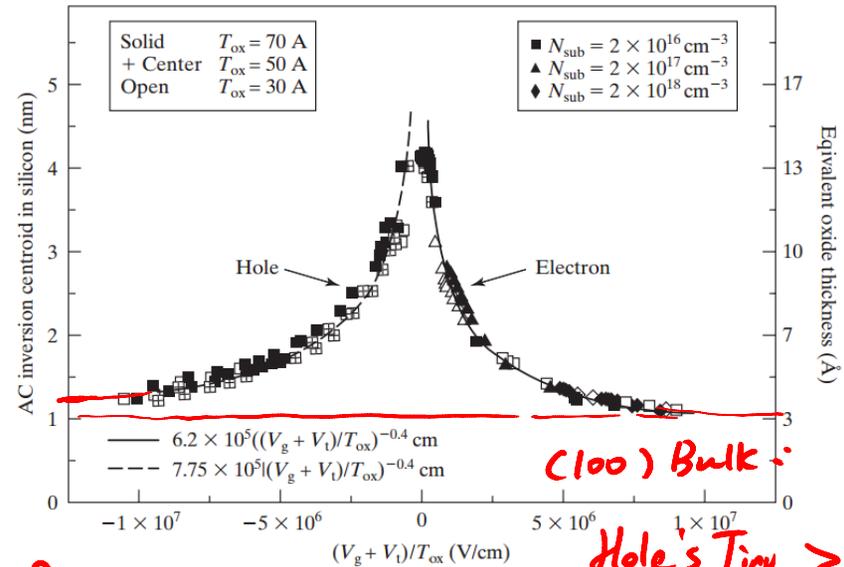
- Inversion Thickness (T_{inv})



- Quantum Capacitance



Measured T_{inv} in Si Bulk CMOSFETs



K. Yang, VLSI-T (1999) *Electron's T_{inv}*

\Rightarrow *Electrostatics poor for PMOS*

Hence there are 3 metrics to characterize C_{gate} ...

- Physical Oxide Thickness (t_{ox})
- Effective Oxide Thickness (EOT)
- Electrical Effective Oxide Thickness (EOT_{elec}) = $EOT + T_{inv} \cdot \frac{\epsilon_{SiO2}}{\epsilon_{Si}}$

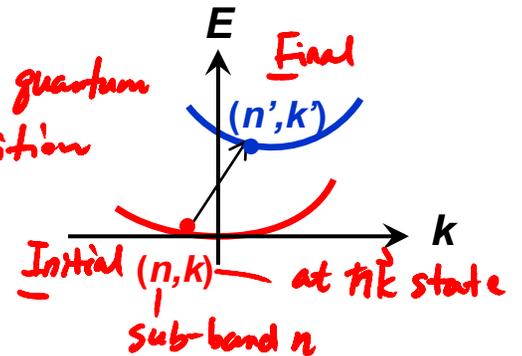
Wave function: $\psi \sim A \cdot \phi^{-i\vec{k} \cdot \vec{r}} \cdot \delta(z)$ → Confined (QW) part, envelop function, representing the spatial distribution

Carrier Mobility: A Quantum Mechanical View

plane wave part (x-y plane):
 $\vec{k} = \vec{k}_x + \vec{k}_y$, $\vec{r} = \vec{x} + \vec{y}$

- Fermi Golden Rule:** transition rates between two quantum states = scattering is a kind of quantum transition

$$S_{n\vec{k}, n'\vec{k}'} = \frac{2\pi}{\hbar} |M(n, \vec{k}, n', \vec{k}')| \cdot \delta(E_n(\vec{k}) - E_{n'}(\vec{k}') \pm \hbar\omega)$$



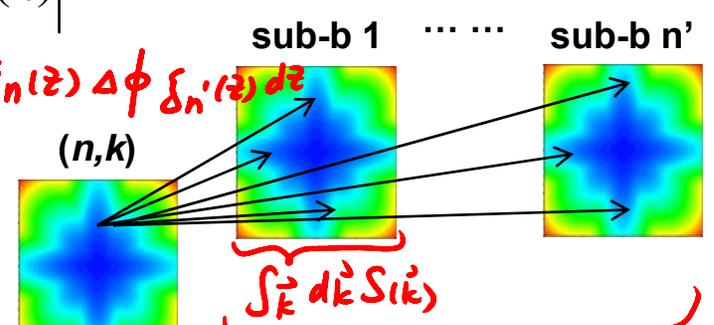
✓ wavefunction overlap along confinement direction $F_{n,n'} = \int dz \cdot |\xi_n(z) \cdot \xi_{n'}^*(z)|^2$

✓ $\Delta\phi$: disturbing (scattering) potentials

- mobility:** scattering-induced quantum state transitions

$|M| \propto \int \xi_n(z) \Delta\phi \xi_{n'}^*(z) dz$

scattering rates for sub-band n at k $\frac{1}{\tau_n(\vec{k})} = \sum_{n'} \int_{\vec{k}'} \frac{d\vec{k}'}{(2\pi)^2} \cdot S_{n\vec{k}, n'\vec{k}'} \times \Phi(n\vec{k}, n'\vec{k}')$



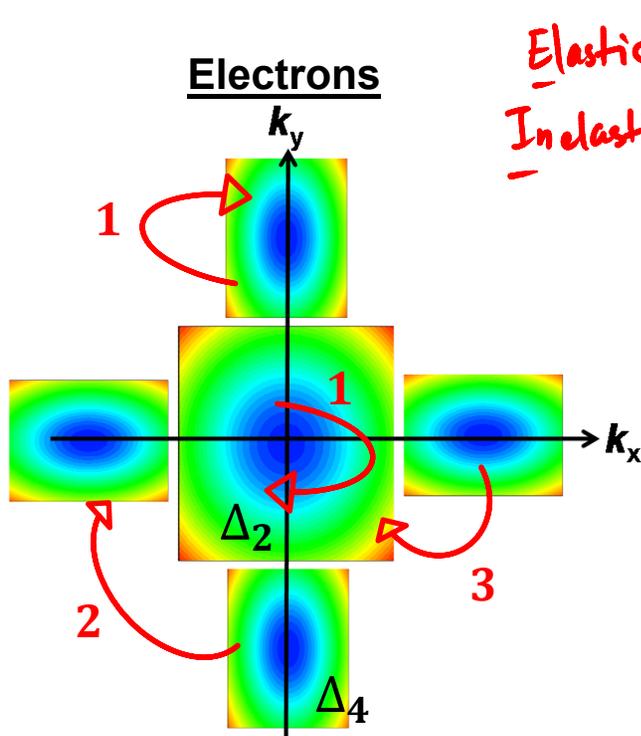
$$\mu_{i,j}^n = \frac{e}{\hbar^2} \cdot \frac{1}{k_B T} \cdot \frac{g_n}{n_n} \int_{\vec{k}} \frac{d\vec{k}}{(2\pi)^2} \cdot \tau_{i,j}^n \cdot \frac{\partial E_n}{\partial k_i} \cdot \frac{\partial E_n}{\partial k_j} \cdot f(E_n) \cdot (1 - f(E_n))$$

for the n^{th} sub-band
Fermi func, carrier's occupation

$$\mu_{i,j}^{\text{tot}} = \frac{1}{n_{\text{tot}}} \sum_n n_n \cdot \mu_{i,j}^n$$

for the overall inversion layer
weighted average by $N_{\text{sub-band}}$

Transition Types of Carriers

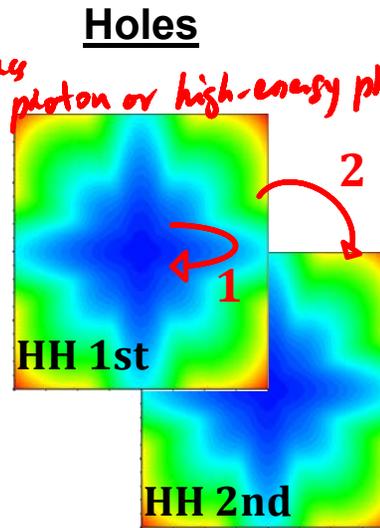


Valley degeneracy:

$\Delta_2: 2$ $\Delta_4: 4$ *both I & E*

- 1. intra-valley scattering *E*
- 2. g-type inter-valley scattering *E*
- 3. f-type inter-valley scattering *I*

Elastic: PE \approx KE
Inelastic: requires $\hbar\omega$ (photon or high-energy phonon)



- 1. intra-sub-band scattering *both I & E*
- 2. Inter-sub-band scattering *E*

$$\frac{1}{\tau_n(\vec{k})} = \sum_{n'} \int_{\vec{k}} \frac{d\vec{k}'}{(2\pi)^2} \cdot S_{n\vec{k}, n'\vec{k}'} \times \Phi(n\vec{k}, n'\vec{k}')$$

Momentum Relaxation Factor

Acoustic and Optical Phonon Scatterings

Acoustic Phonon Scattering

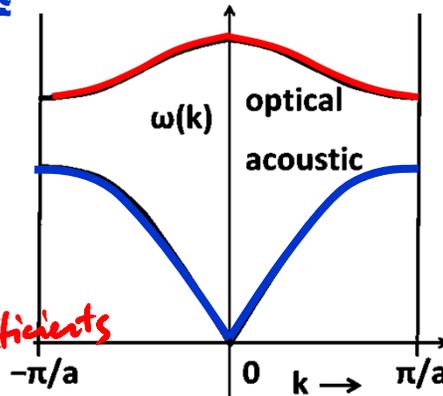
AP: coherent movements of atoms, *i.e.* adjacent atoms move together.



elastic scattering

piezoelectric coefficients

$$M_{elast.}(n, \vec{k}, n', \vec{k}') = \frac{\propto T}{\rho u_l^2} \cdot F_{n, \vec{k}, n', \vec{k}'} \cdot (k_B T \Xi^2)$$



Optical Phonon Scattering

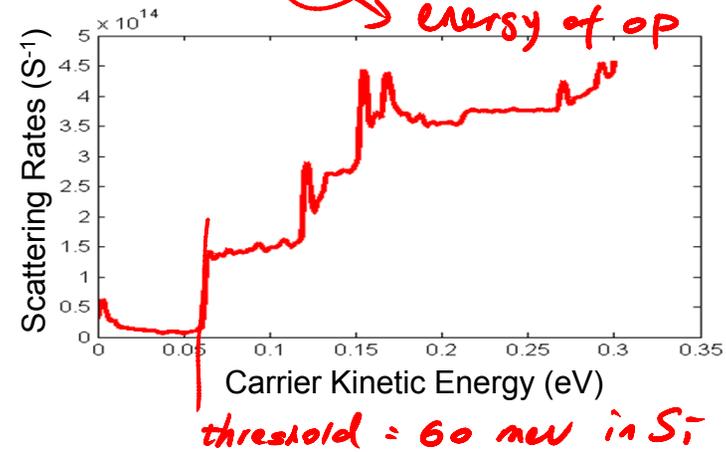
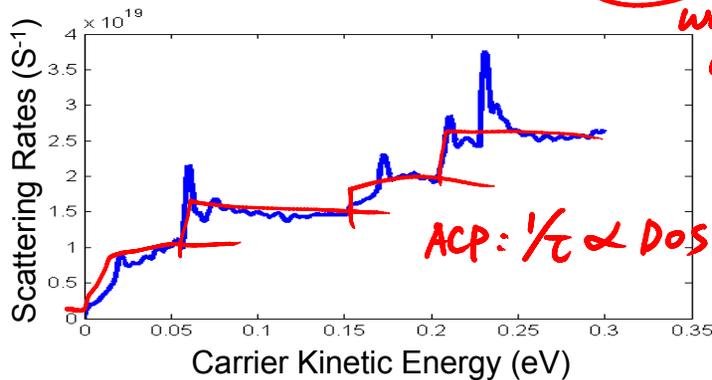
OP: out-of-phase movements of atoms, *i.e.* adjacent atoms move in opposite directions.



inelastic scattering

of OP

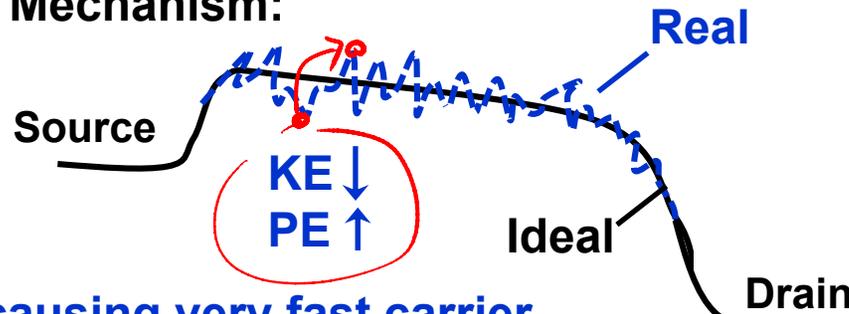
$$M_{inelast.}(n, \vec{k}, n', \vec{k}') = \frac{\hbar^2 \pi (D_l k)^2}{2\rho(\hbar\omega)} \cdot F_{n, \vec{k}, n', \vec{k}'} \cdot \left(n_{op}(\hbar\omega) + \frac{1}{2} \mp \frac{1}{2} \right)$$



Surface Roughness Scattering

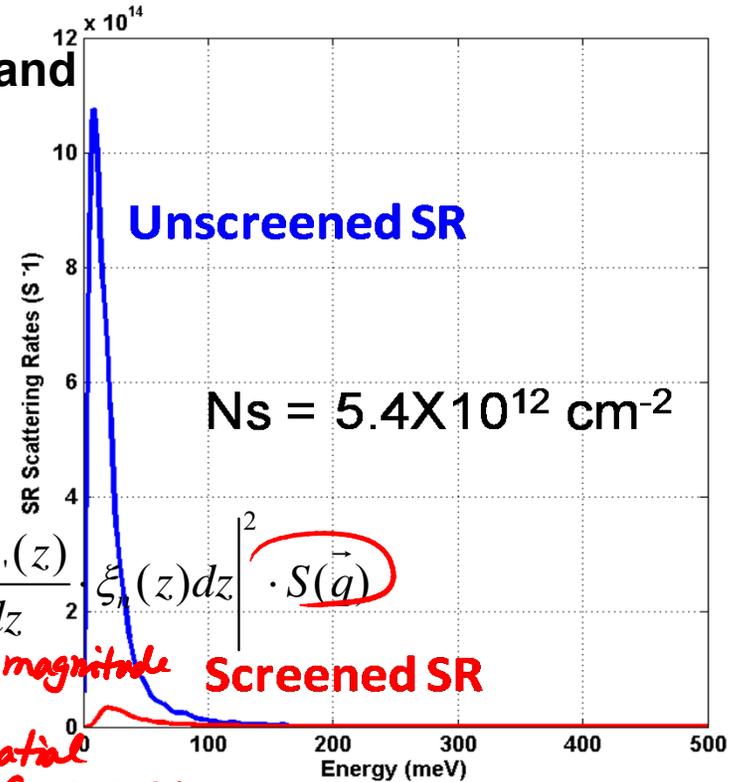
L. Donetti, JAP (2009)

- Type: elastic scattering, mostly intra-valley/band
- Mechanism:



causing very fast carrier momentum change!

"Effective" \vec{E} -field seen by carriers E_c



$$M_{surf.rough.}(n, \vec{k}, n', \vec{k}') = \left| \int_z \xi_n(z) \cdot \vec{E} \cdot \xi_{n'}(z) dz + (E_n^0 - E_{n'}^0) \int_z \frac{d\xi_{n'}(z)}{dz} \xi_n(z) dz \right|^2 \cdot S(\vec{q})$$

Power Spectrum of Surface Roughness

$$S(\vec{q}) = \frac{\pi(\Delta\lambda)^2}{[1 + (q\lambda)^2/2]^{3/2}}$$

Δ : SR magnitude
 λ : spatial frequency

Considering screening effect (important at high gate voltage):

$$\left| M_{screen}(n, \vec{k}, n', \vec{k}') \right|^2 = \frac{\left| M_{unscr.}(n, \vec{k}, n', \vec{k}') \right|^2}{\epsilon^2(\vec{q})}$$

at low N_{inv} , $\epsilon \rightarrow 11.7$ (Si)
at high N_{inv} , $\epsilon \rightarrow \infty$

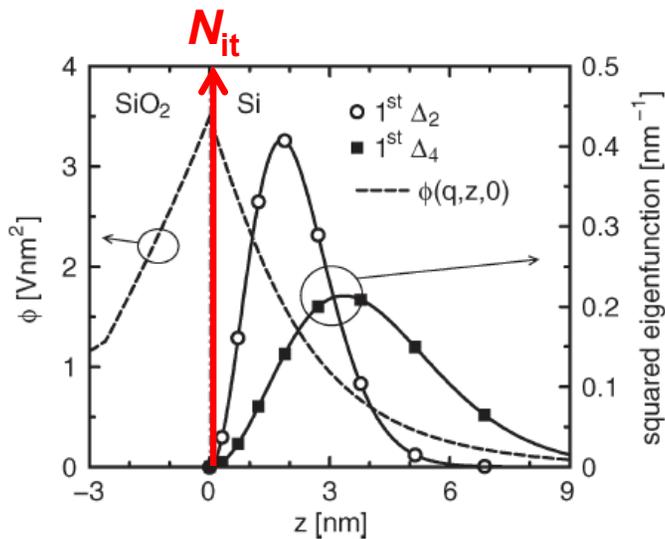
Dielectric function

Coulomb Scatterings

- Type: elastic scattering, mostly intra-band/valley → *small δk change during scatterings*
- Mechanism:

$$\phi_{unscr}(\vec{q}, z) = \frac{e}{\vec{q}(\epsilon_{Si} + \epsilon_{ox})} e^{-\vec{q}|z|} \quad M_{n,n'}(\vec{q}, z_0) = \frac{e}{A} \int_0^\infty \phi(\vec{q}, z, z_0) \xi_n(z) \xi_{n'}(z) dz$$

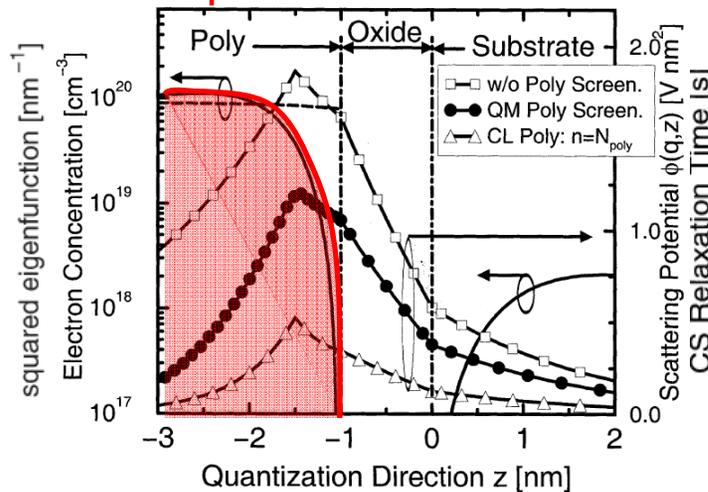
SiO₂/Si Interface Charge



F. Driussi, TED (2009)

Depletion Charge

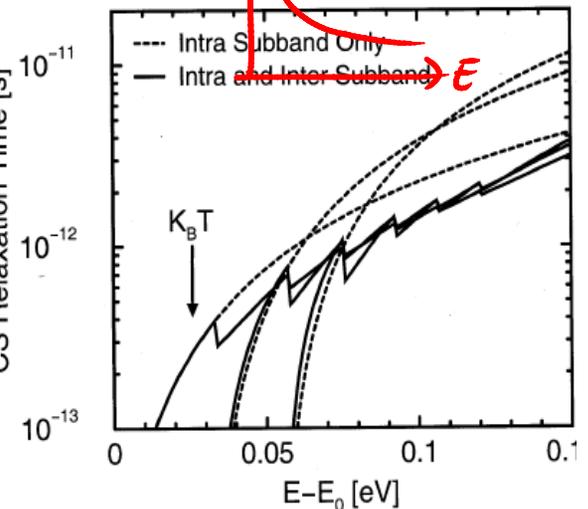
Q_{dep} in poly-si & bulk



D. Esseni, TED (2003)

MRT (1/Scattering Rates)

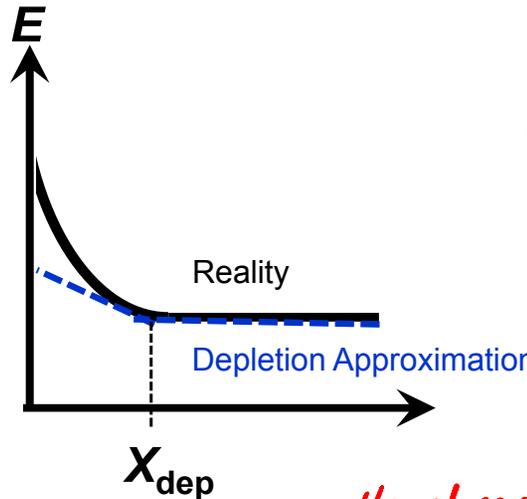
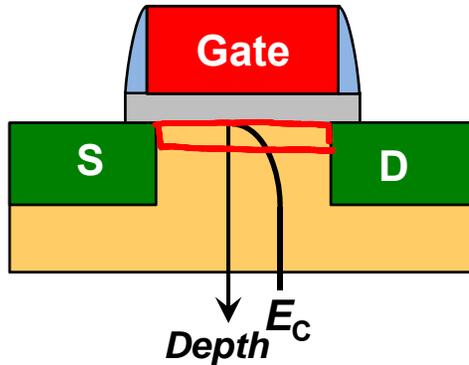
→ 1/ε ↑



F. Driussi, TED (2009)

Effective Transverse Field (E_{eff})

In a MOS Inversion Layer:



2D Sheet Charge Density:

$$Q_{inv} = \int_0^{T_{inv}} qn(x)dx$$

$$Q_{dep} = \int_0^{X_{dep}} qN_B(x)dx$$

Surface (oxide/Si interface) field:

$$E_s = \frac{Q_{dep} + Q_{inv}}{\epsilon_{Si}}$$

Bottom (of inversion layer) field:

$$E_b = \frac{Q_{dep}}{\epsilon_{Si}}$$

Average field:

$$E_{ave} = \frac{E_s + E_b}{2} = \frac{Q_{dep} + Q_{inv}/2}{\epsilon_{Si}} \equiv E_{eff}$$

More generally:

$$E_{eff} = \frac{Q_{dep} + \alpha \cdot Q_{inv}}{\epsilon_{Si}}$$

fitting para.

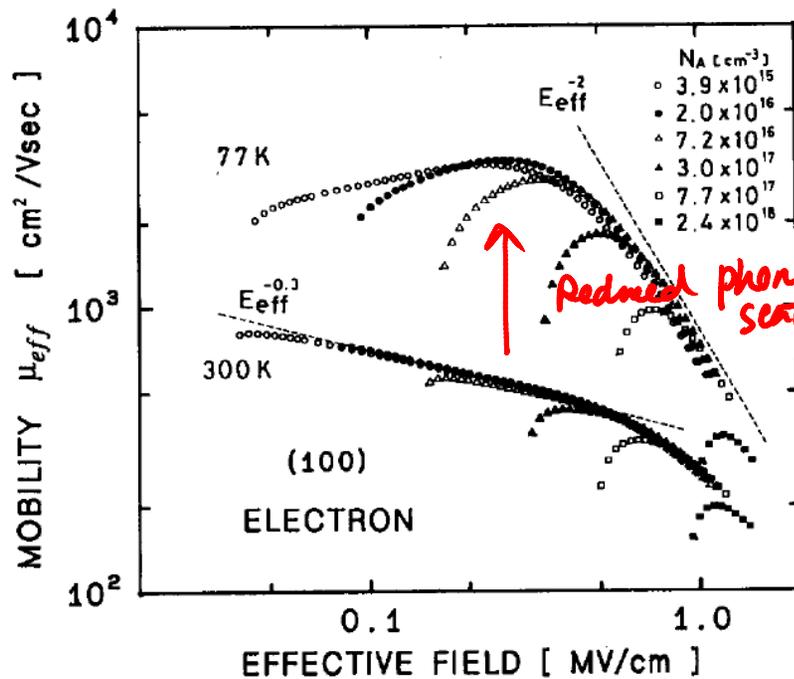
the closer inversion charge to ox/si interface (i.e. the smaller T_{inv}) is, the larger α value will be.

For (100) bulk Si MOSFET:
 Electrons: $\alpha = 0.5$
 Holes: $\alpha = 0.33$

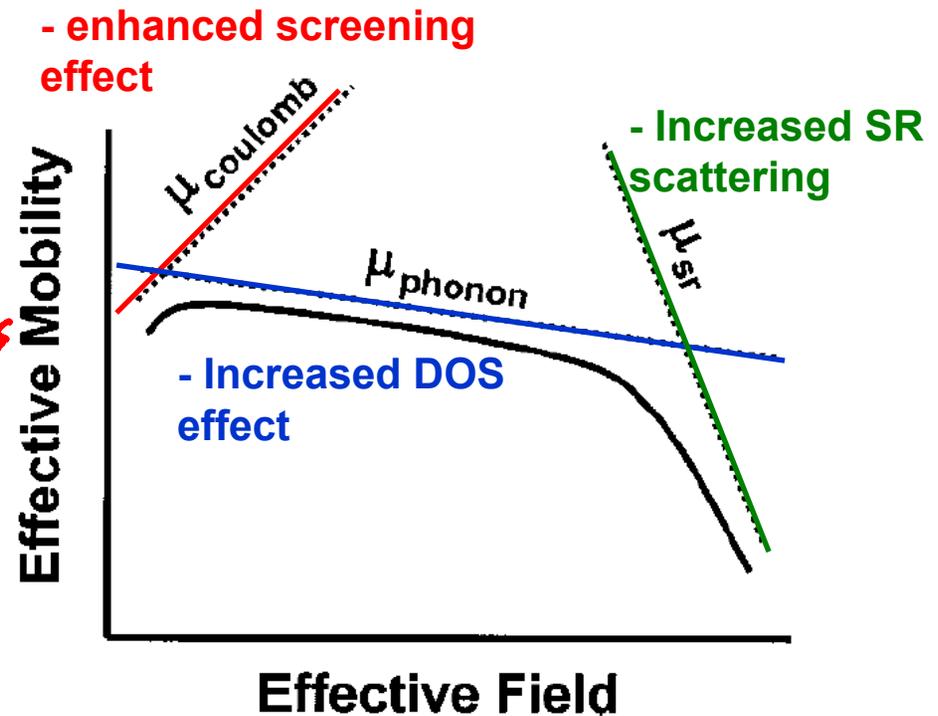
Universal Mobility Curve: μ vs. E_{eff}

- Unify the electric field value by including the oxide thickness (compared to μ vs. V_G) and depletion charge effect (compared to μ vs. N_{inv}).

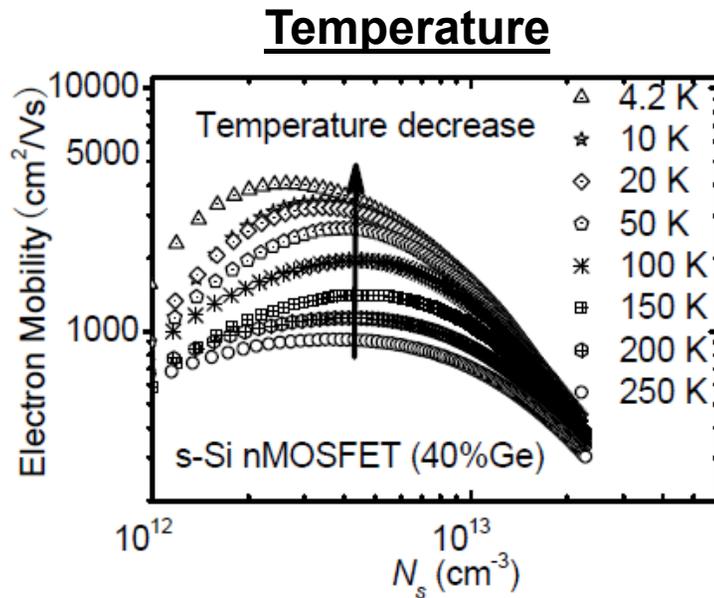
Measured Si Universal Curves



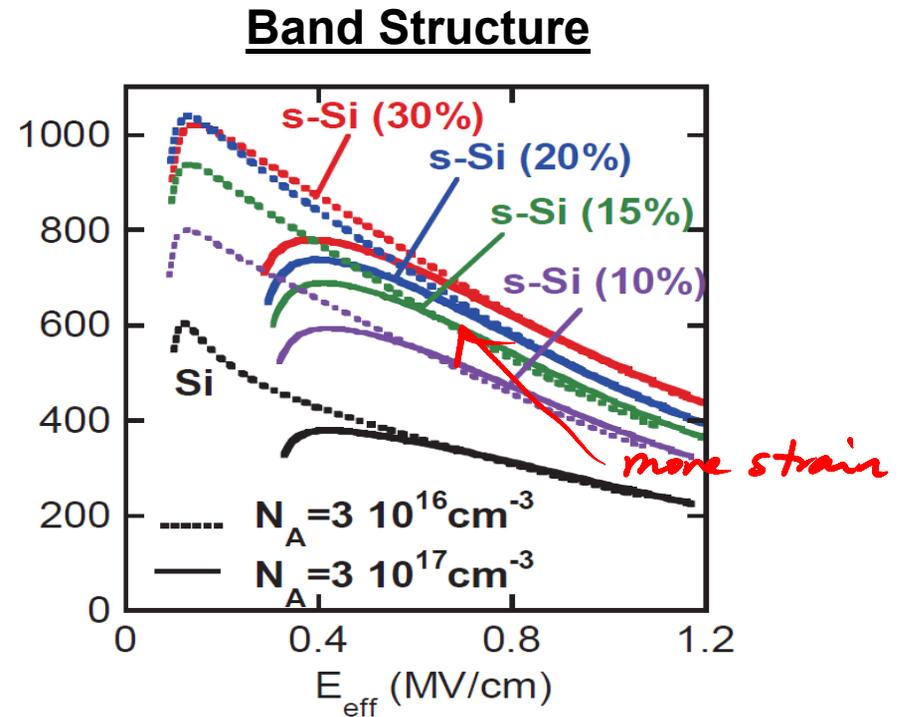
S. Takagi, TED (1994)



Universal Mobility Curve: Dependent Factors



Y. Zhao, IEDM (2008)

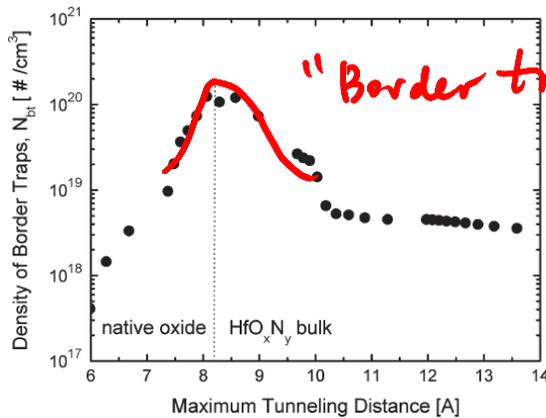


O. Weber, VLSI-T (2007)

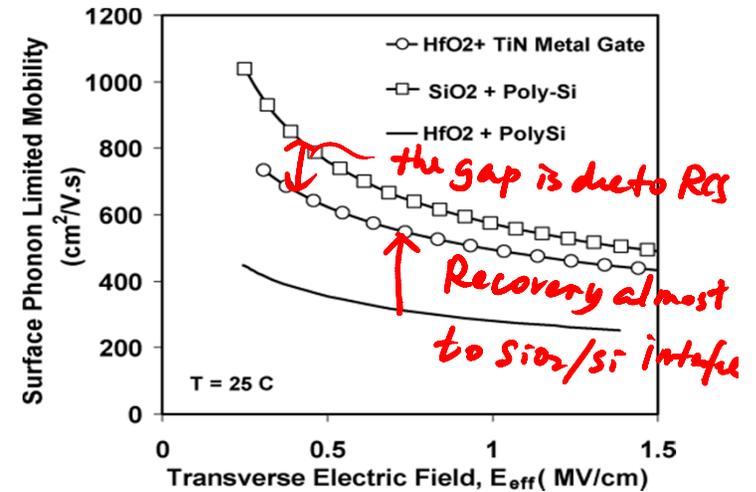
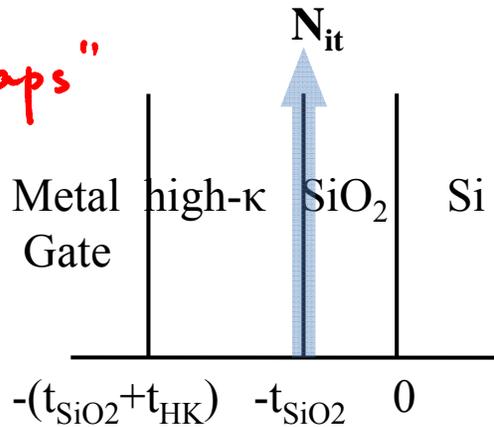
- Si universal mobility curves are often used to show a new technology's enhancement.

High-κ-induced Scatterings

- Remote Coulomb Scattering

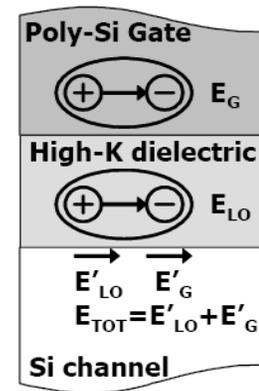
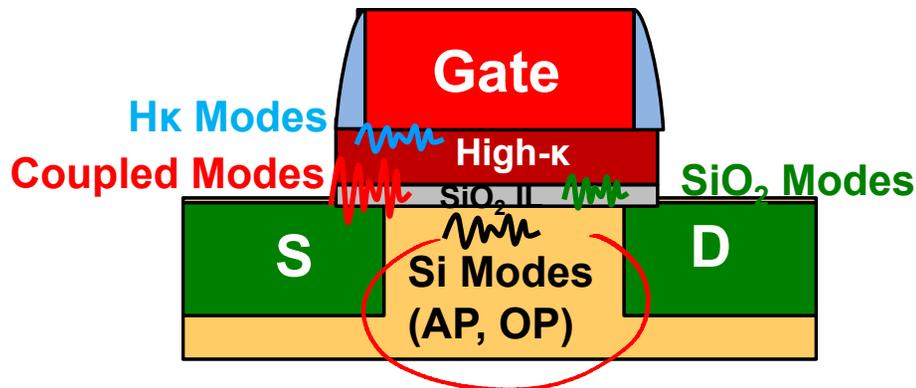


C.-Y. Lu, EDL (2006)

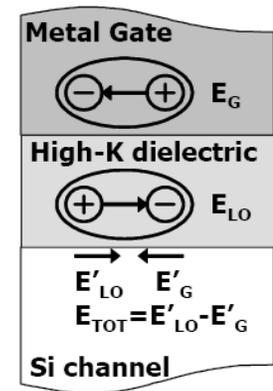


R. Chau, EDL (2004)

- Remote (Surface Optical) Phonon Scatterings



(a) In resonance



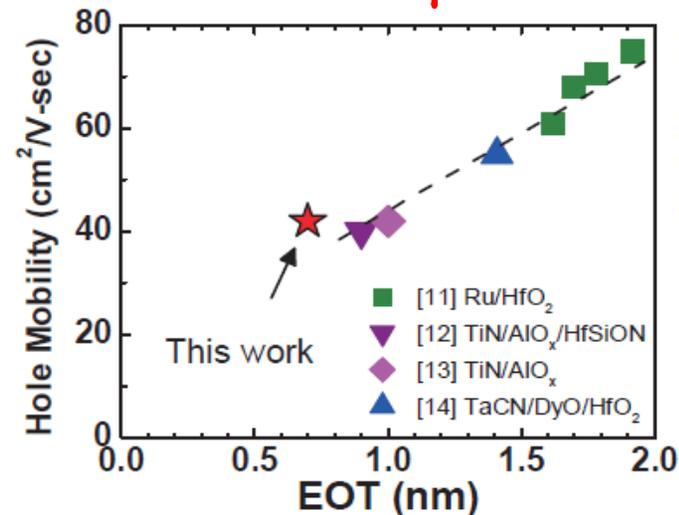
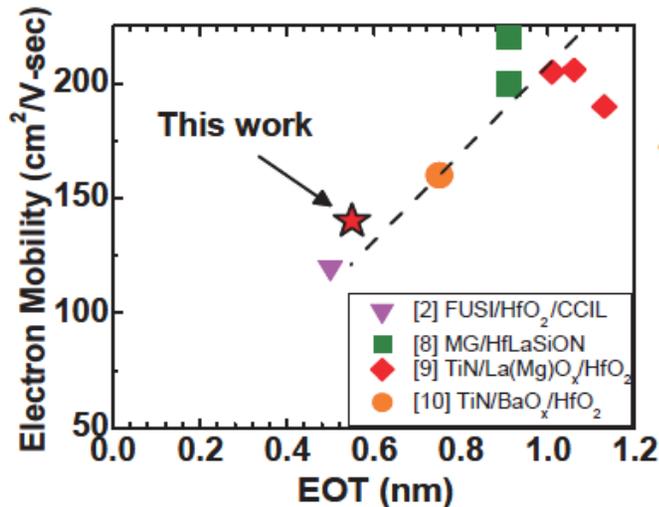
(b) Off resonance

Courtesy of D. Vesileska (ASU)

Dependence of High- κ Thickness $C_{ox} \propto \frac{1}{EOT}$

- Mobility doesn't follow universal curve.

$I_m \propto C_{ox} \cdot \mu_{eff}$, since $\mu_{eff} \propto EOT$
 trade-off \uparrow

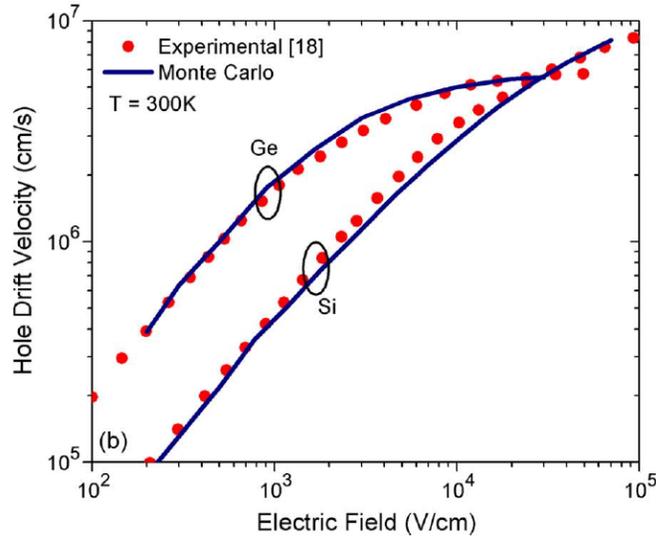


K. Choi, VLSI-T (2009)

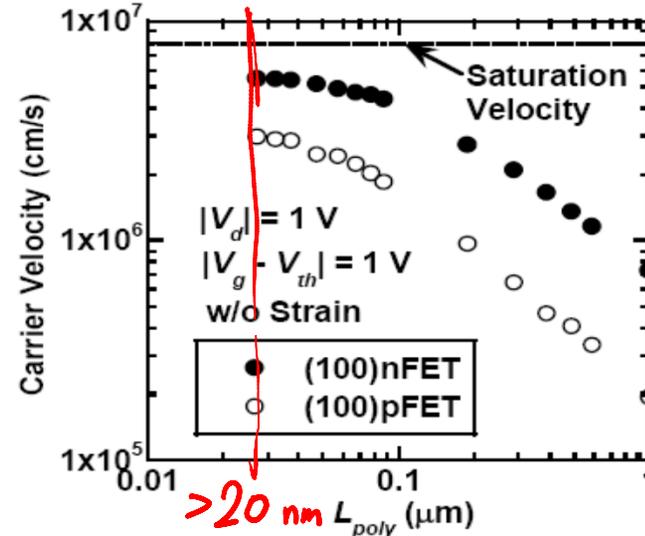
- By using metal-gate technology, RCS becomes the limiting factor in state-of-the-art MOSFET's mobility.

Si Carrier Velocity Saturation

- Under high lateral electric field, carrier velocity saturates to a constant value, due to dramatically enhanced optical phonon scatterings.



B. Ho, TED (2011)



M. Saitoh, IEDM (2009)

- State-of-the-art technologies actually pushes away MOSFETs from *being* velocity saturation, due to:

- Increased doping/junction defects - $\mu \downarrow$
- High- κ -induced scatterings
- Ballistic transport (will be discussed in Lec. 5) *reduced scattering events*
- Reduced V_{DD} *reduced $\vec{E}_{lateral}$*

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