

# Development of Efficient Inelastic Scattering in Atomistic Tight Binding

## Master's Defense

James Charles

Network for Computational Nanotechnology  
(NCN)

Electrical and Computer Engineering

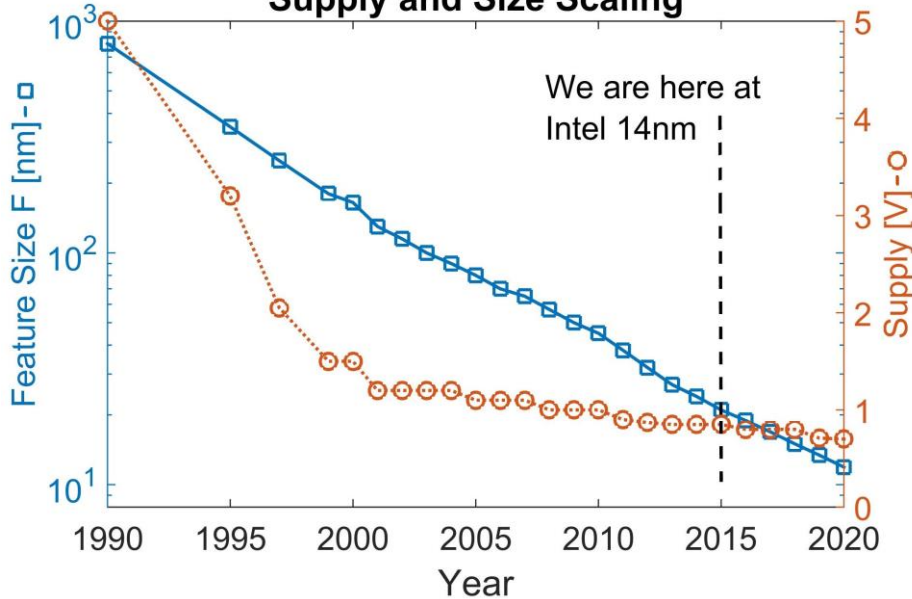
[charlesj@purdue.edu](mailto:charlesj@purdue.edu)

1. Motivation
2. Acoustic and Optical Phonon Scattering Verification
3. Effect of scattering on MOSFETs
4. Effect of scattering on TFETs
5. Why does scattering increase tunneling current?
6. Numerical Details
7. Conclusions/Future Work

- 1) Motivation
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Figure courtesy of Tarek Ameen

## Supply and Size Scaling

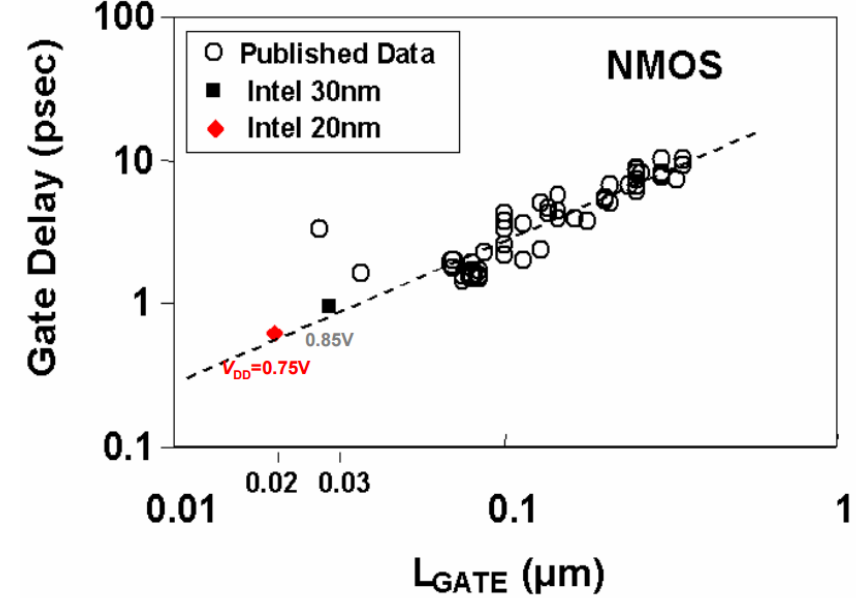


### Length Scaling:

- 1) Area  $\checkmark$  transistor density  $\nearrow$
- 2) Capacitance  $\checkmark$  Delay  $\checkmark$

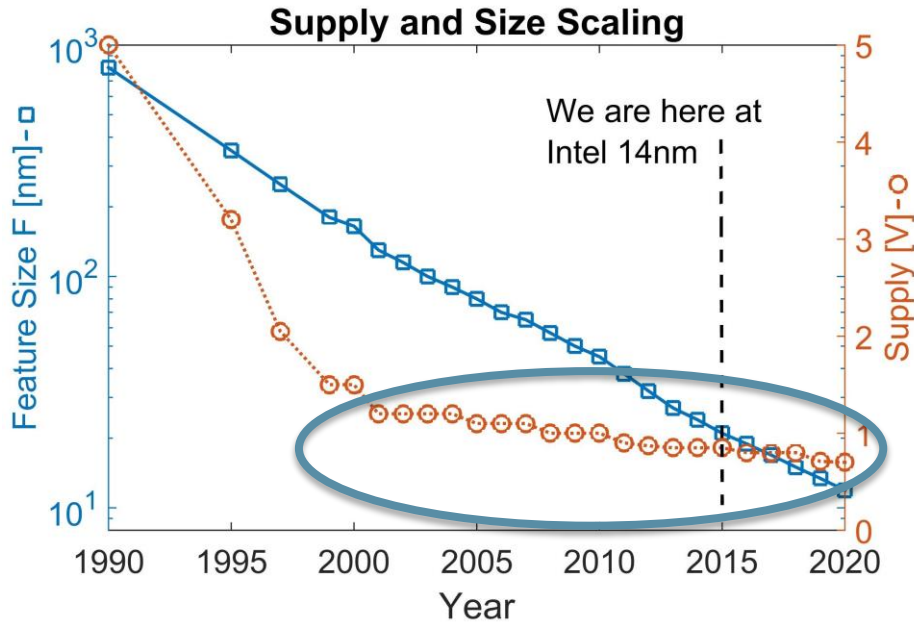
$$\text{Gate Delay} \propto C_{gate} V_{DD} / I_{sat}$$

<http://www-inst.eecs.berkeley.edu/~ee40/fa03>



Length continues to scale smoothly

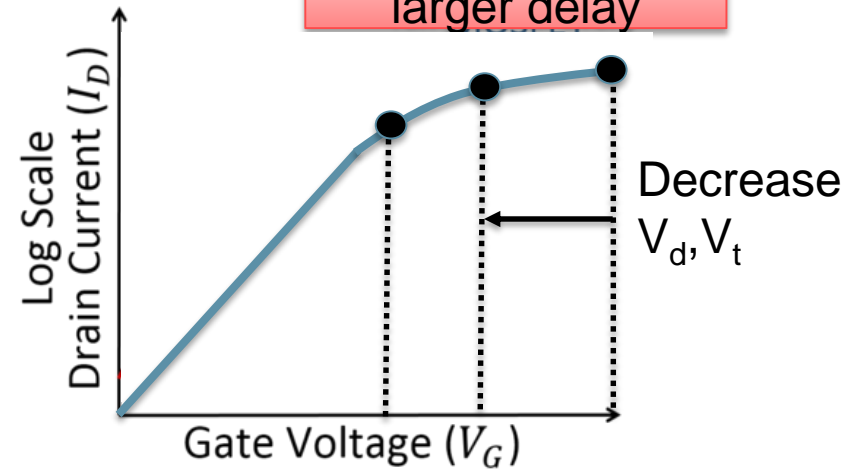
Figure courtesy of Tarek Ameen



Why has voltage scaling saturated around 2000?

$$\text{Gate Delay} \propto C_{gate} V_{DD} / I_{sat}$$

$I_{sat}$  decreases, larger delay



Keep off-current constant

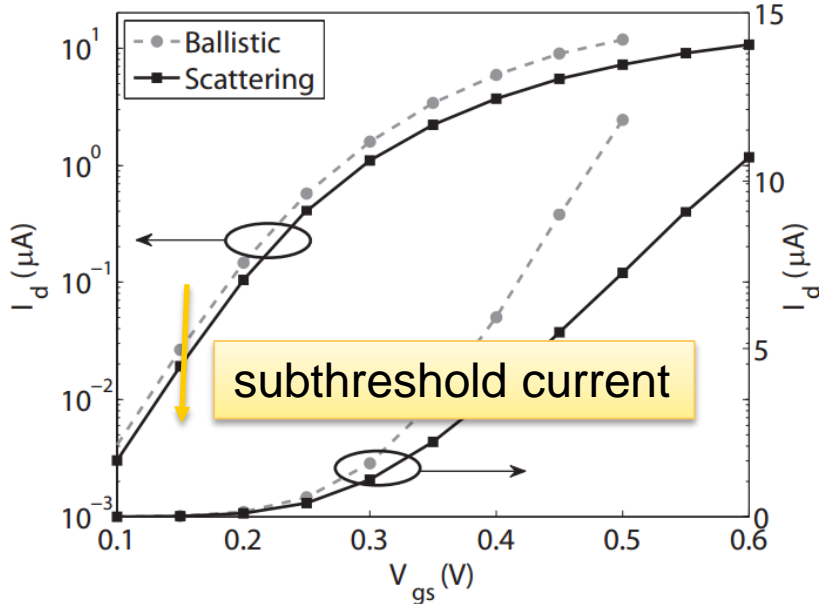
**Voltage Scaling:**

- ✓ Static Power  $\propto V_{DD} I_{off}$
- ✓ Dynamic Power  $\propto V_{DD}^2$

Voltage scaling has saturated

“that the **reduction [compared to ballistic]** of the device drain current, ...is more important in the ON-state than in the OFF-state of the transistor”

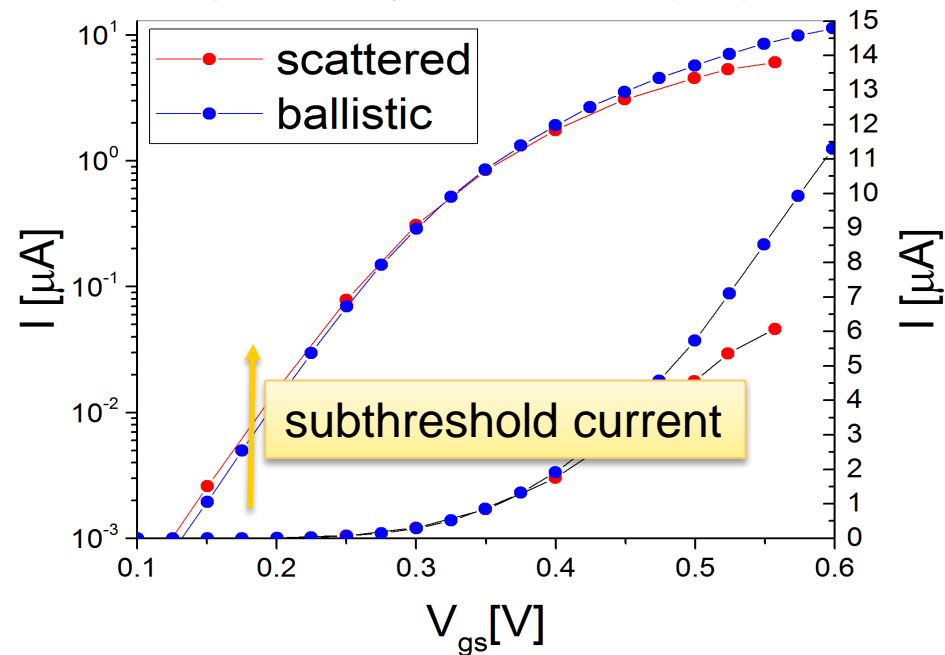
M. Luisier and G. Klimeck Phys. Rev. B **80**, 155430 (2009).



3 nm circular silicon nanowire,  $V_{ds} = 0.6V$   
 $sp^3d^5s^*$  tight binding basis  
 confined phonon model

ballistic yields an **underestimation** of the subthreshold current up to 20%

Data from A. Esposito, M. Frey, et. al. JCEL vol. 8 (2009).



3.2 nm square silicon nanowire,  $V_{ds} = 0.5V$   
 non-parabolic effective mass basis  
 bulk phonon model

Conflicting trends for subthreshold current in literature. How to resolve this?

## Critical Questions:

- 1) How to increase electrostatic gate control?
- 2) What is the limit of gate length scaling?
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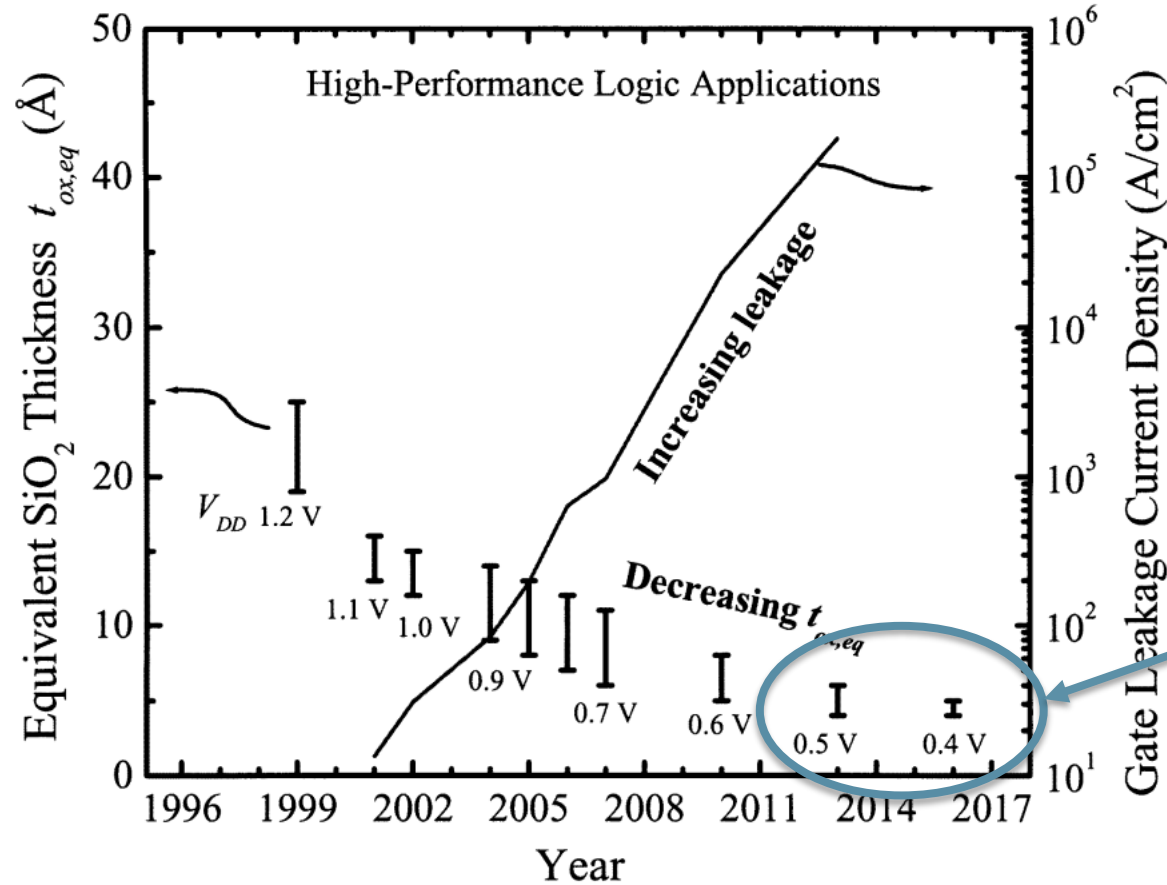
## Critical Questions:

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↗ capacitance ↘ oxide thickness

↗ gate leakage

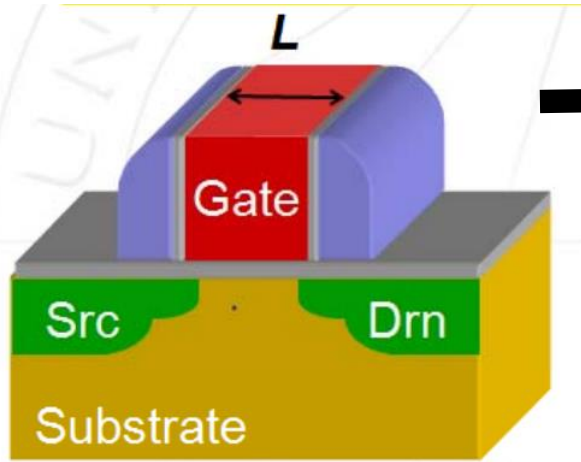


Oxide scaling is saturated

Leakage puts a limit on minimum oxide thickness

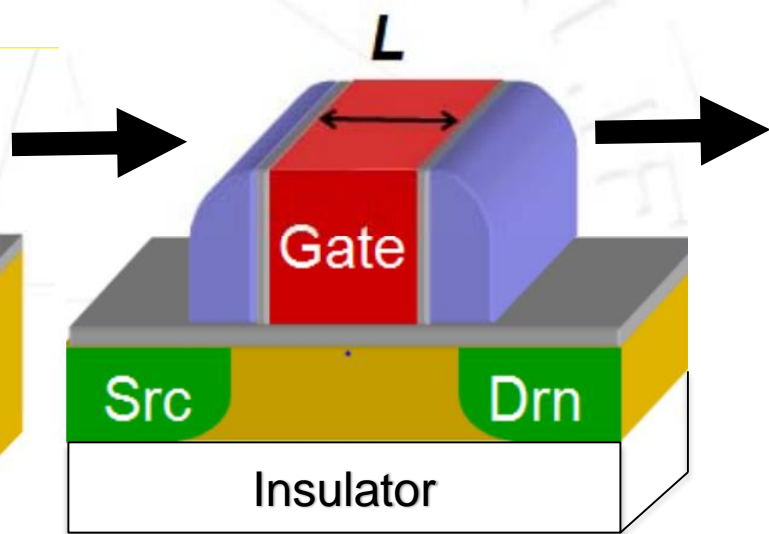
### Geometry Trend

increased electrostatic control

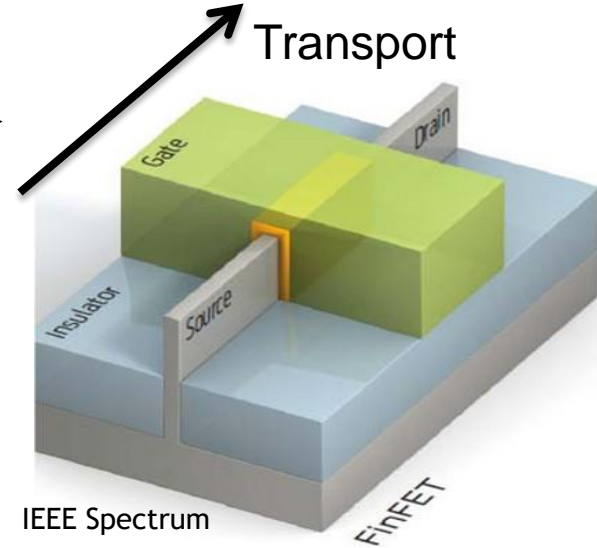


Bulk

ESSDERC 2012



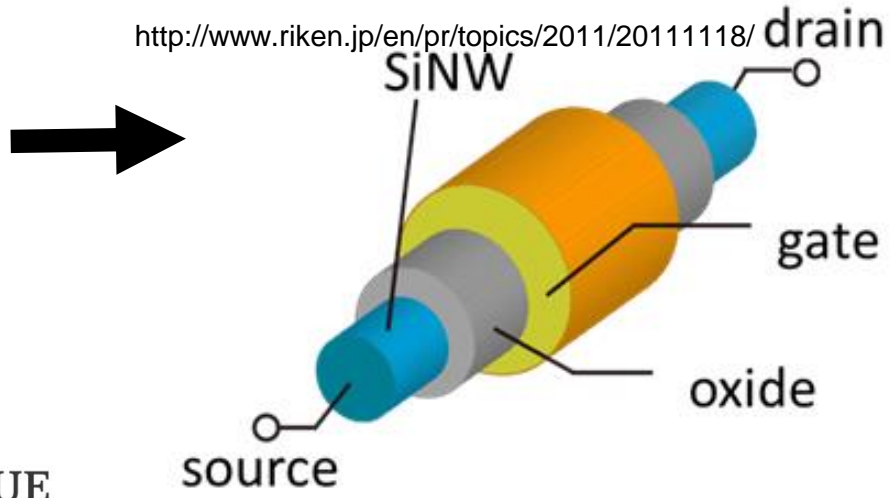
SOI



IEEE Spectrum

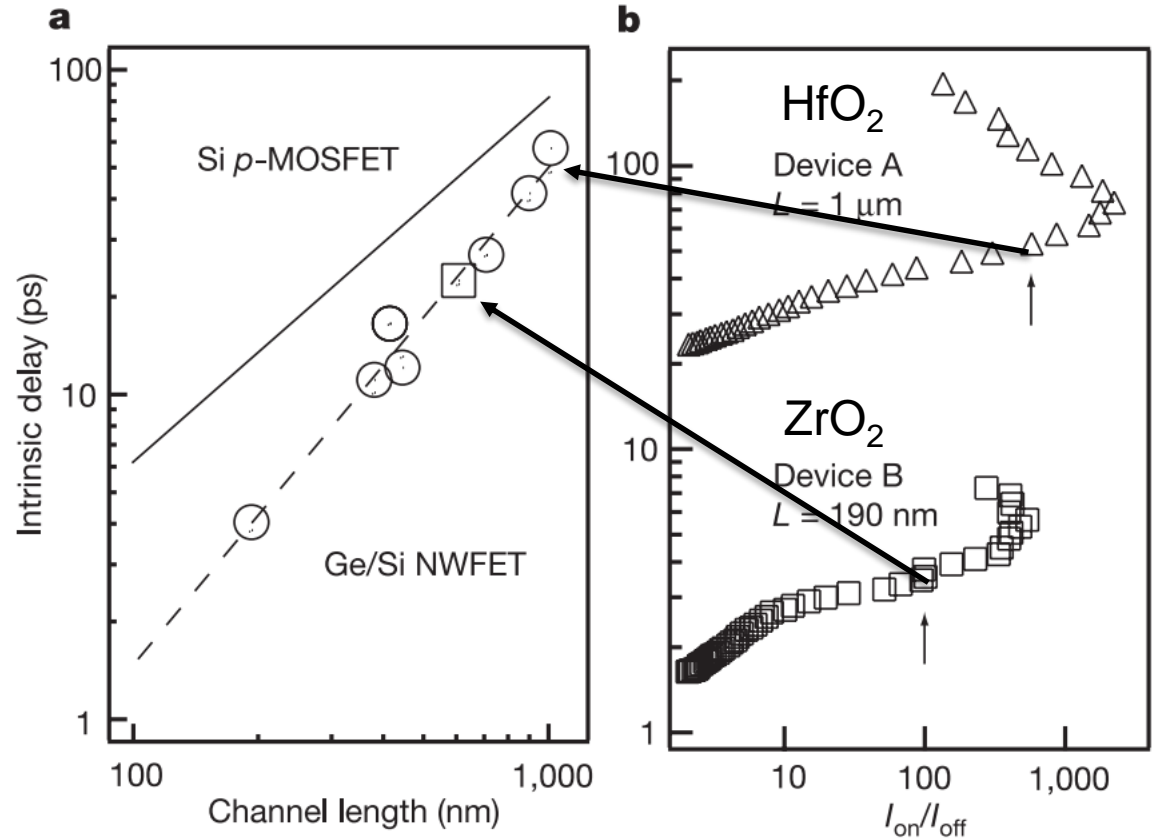
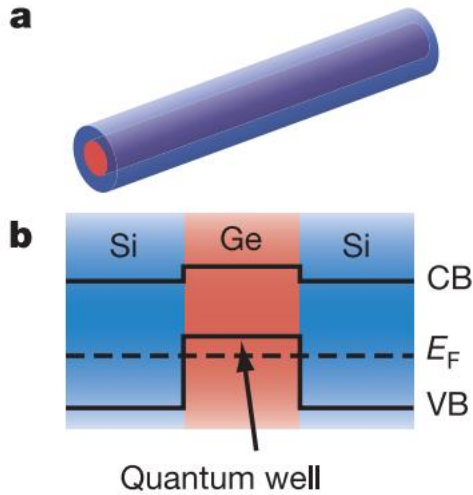
FinFET

<http://www.riken.jp/en/pr/topics/2011/20111118/>



Nanowires candidate for best electrostatic control

J. Xiang Nature Vol. 441 (2006).

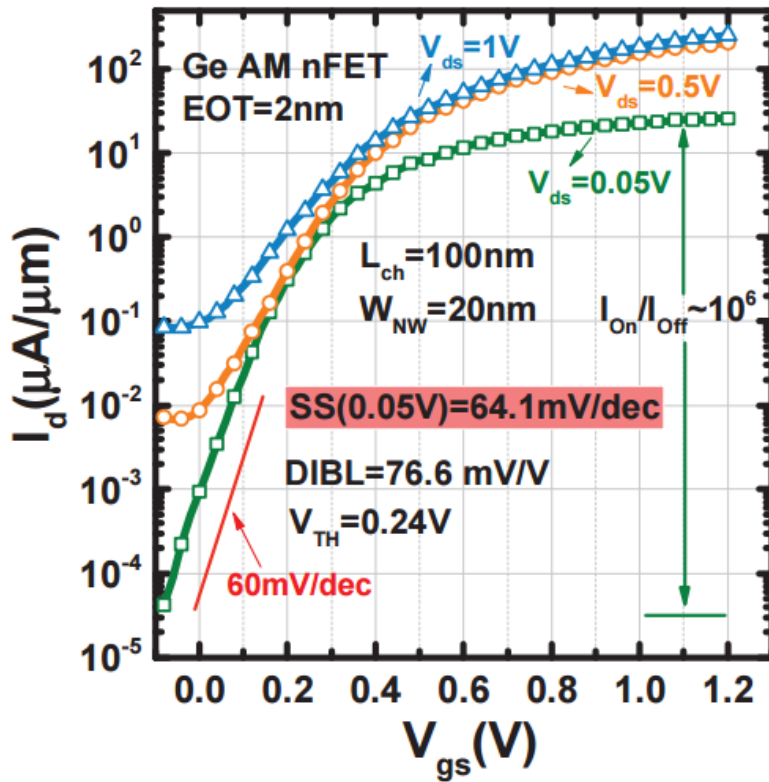


Nanowire increased drive current and reduced delay

p-MOSFET data from Chau, R. *et al.* Benchmarking nanotechnology for high-performance and low-power logic transistor applications. *IEEE Trans. Nanotechnol.* **4**, 153–158 (2005).

Experimental evidence of nearly perfect S.S achieved for nanowires

Peide Ye IEDM 2015



“delivering more than 30% and 40% reduced SS over FinFETs and planar MOSFETS”

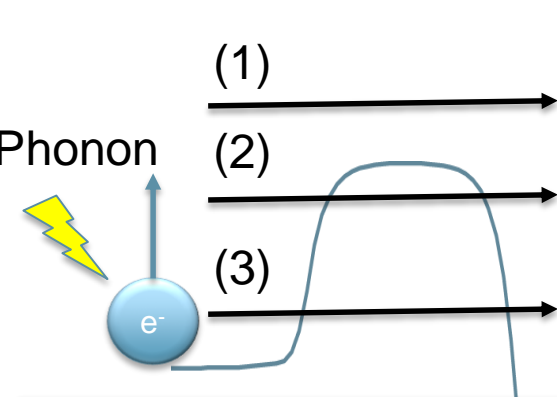
nanowires have excellent gate control

## Critical Questions:

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## ITRS demands scaling of gate length

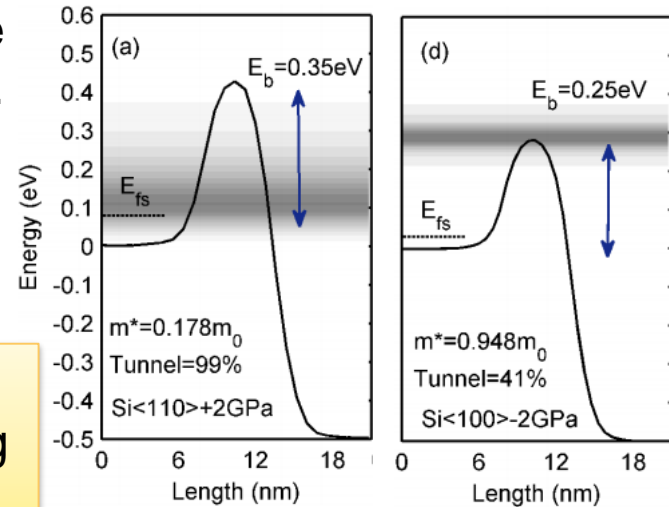
J. Wang, M. Lundstrom, IEDM 2002: "The results show that source-to-drain tunneling does set an ultimate scaling limit"



- (1) Thermionic
- (2) Thermally assisted source-to-drain tunneling
- (3) Direct source-to-drain tunneling

Bandgap engineering shown to decrease tunneling leakage..

S. Mehrota et. al. IEEE Trans. Vol. 60, No.7 (2013).

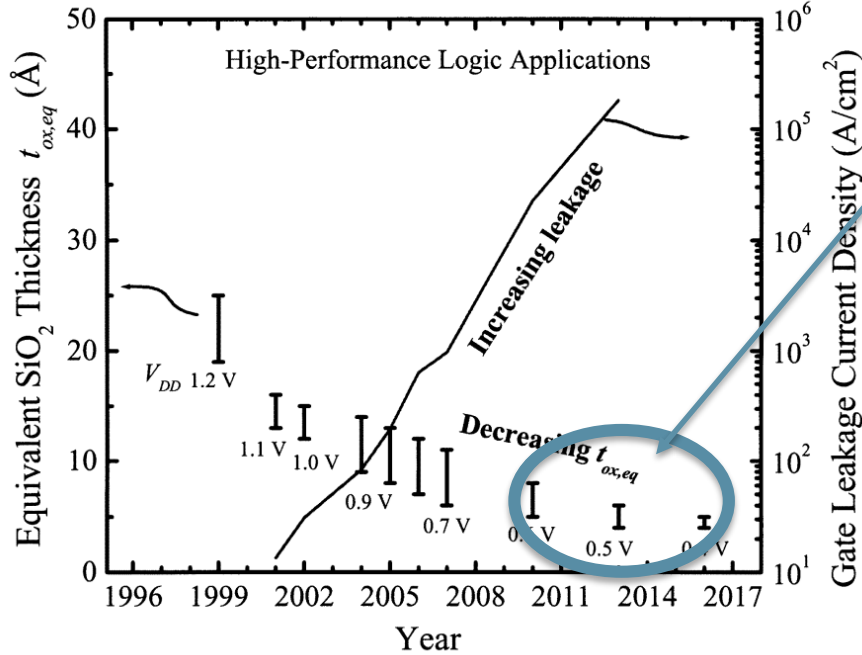


Need to include scattering to account for thermally assisted source-to-drain tunneling

## Critical Questions:

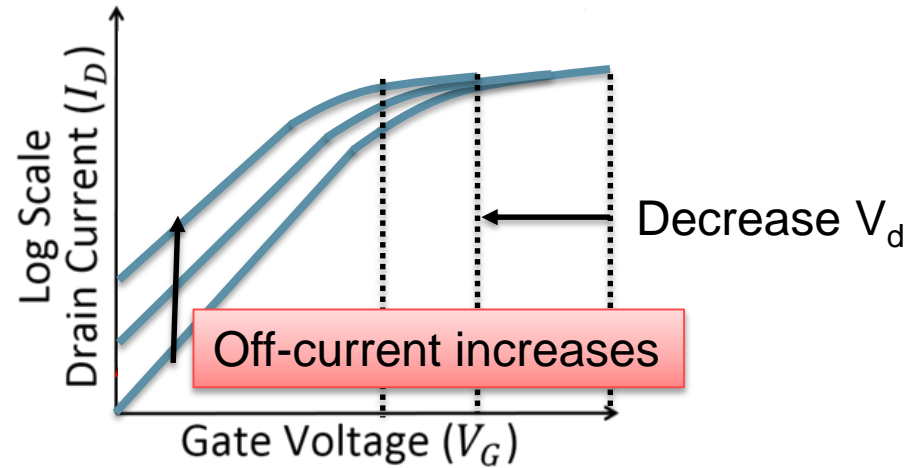
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IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 50,  
NO. 4, APRIL 2003



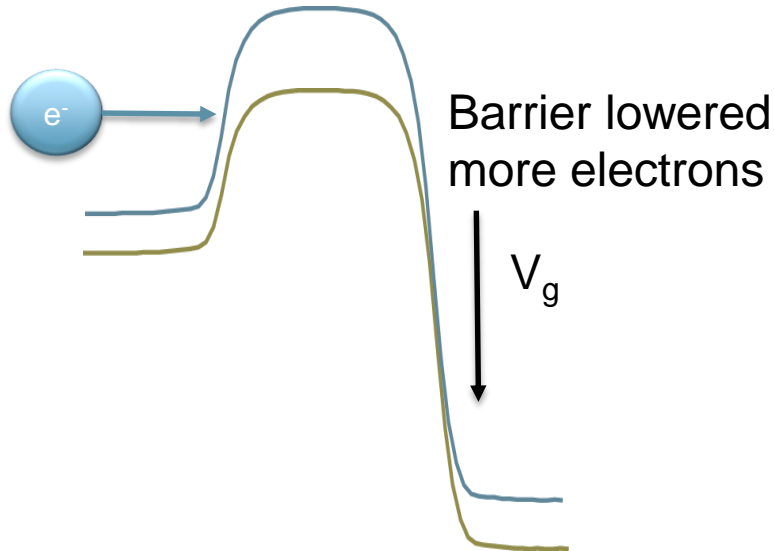
Note: prediction of EOT depends on scaled voltage (dictated by ITRS)

Reality:  
Since ~2000, supply voltage is no longer scaling. Why?





Typical MOSFETs :  
Barrier controlled device



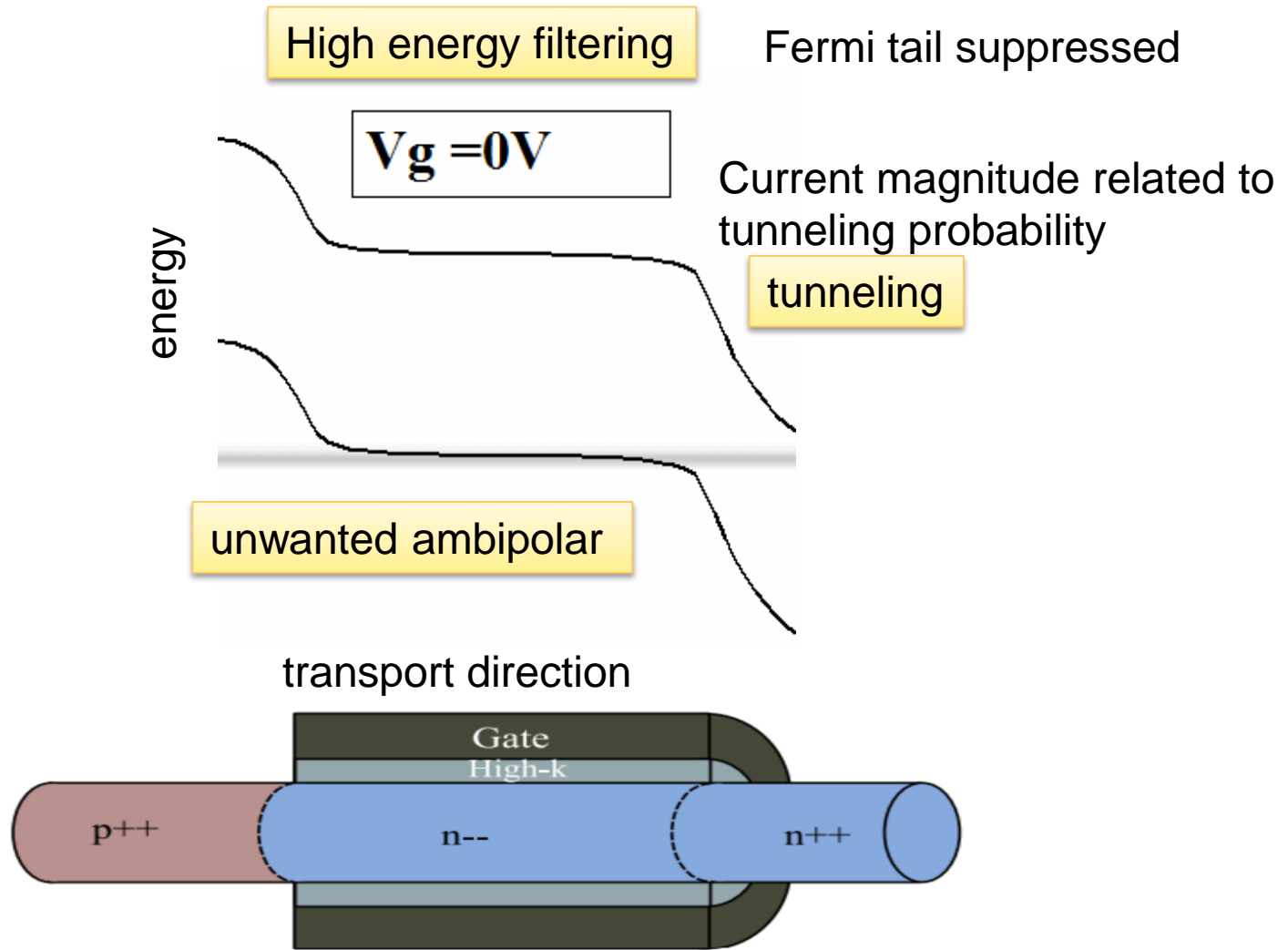
- Sub-threshold slope: fundamental limit of how fast the device can turn on
- This is limited by the Fermi band-tail

$$S.S = \ln(10) \frac{kT}{q} \left( 1 + \frac{C_{ch}}{C_{ox}} \right)$$

$$\min(S.S) = 60 \text{ mV/dec}$$

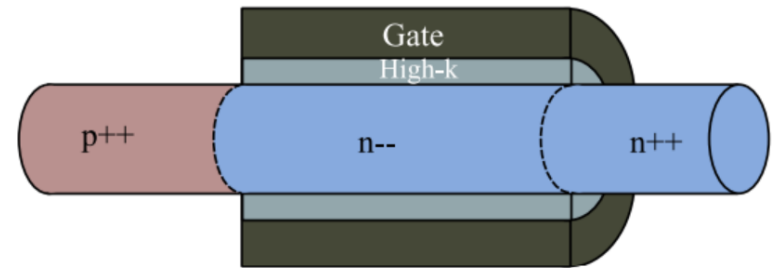
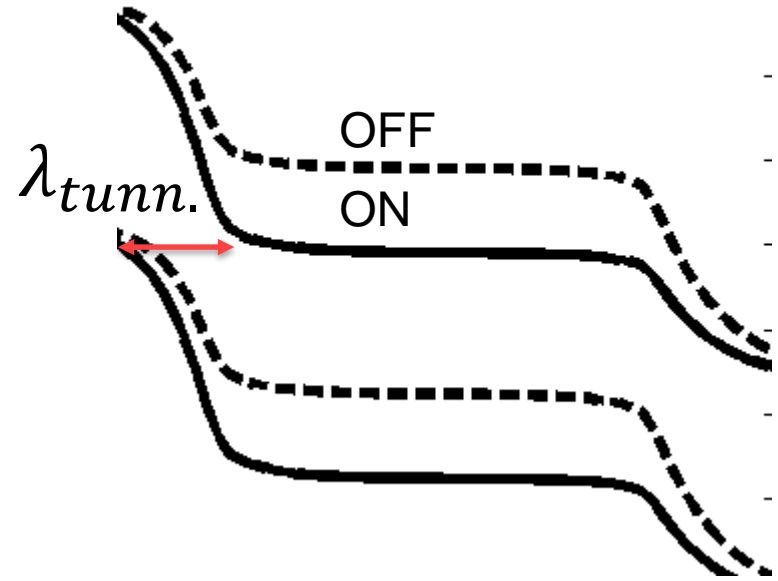
How can we overcome this limit?

## Spectral current for InAs TFET



### Gate-all-around (GAA) nanowire TFET

1. Excellent Gate Control  
 $I_{on}$  increases with steeper source to channel transition  
 (decreased tunneling distance  $\lambda_{tunn.}$ )
2. Best subthreshold-slope compared to MOSFET



What is the importance of scattering in TFETs?

## Critical Questions:

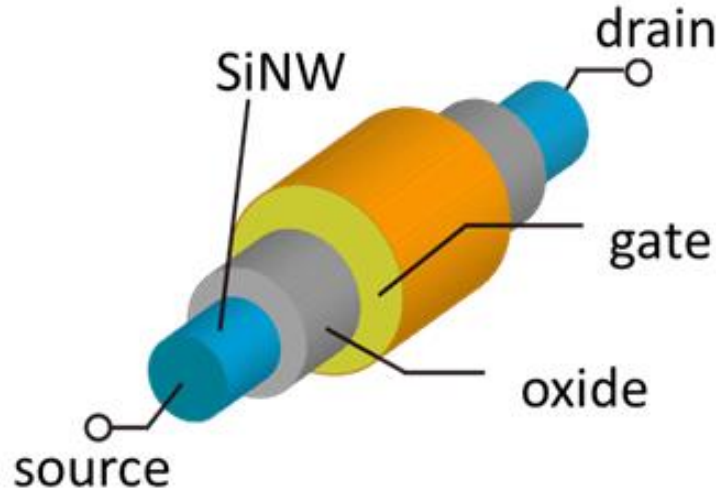
- 1) How to increase electrostatic gate control?
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Method:

Non-equilibrium Green's Function (NEGF) + scattering in the Self-consistent Born Approximation (SCBA)

Atomistic Resolution with Semi-empirical tight binding

<http://www.riken.jp/en/pr/topics/2011/20111118/>



Schematic of Gate All Around (GAA) Nanowire

What is a scattering self-energy?

- Contribution to particle's energy due to interaction with the system.

- Complex matrix

Real Part  $\Sigma^R \sim \Delta E$

Imaginary Part  $\Sigma^R \sim$  related to lifetime of particle.

What is self-consistent Born?

- Interactions treated as (weak) perturbations
- Leads to self-consistent loop to stabilize charge/current

Why include scattering?

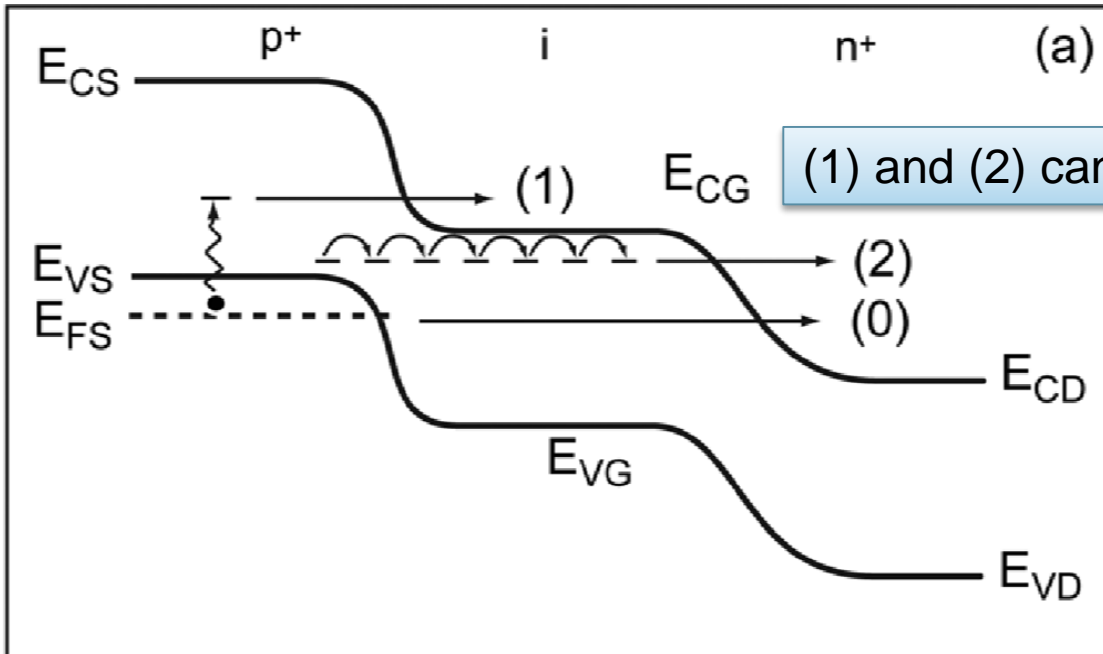
Three Major Effects from scattering :

- Resistive (decreases on-current)
- Increases tunneling current
- Broadens/fills resonant states

### Tunneling mechanisms for TFET

- (0) Direct, coherent tunneling
- (1) Thermally excited carriers tunneling
- (2) Tunneling via channel band-tails

Khayer, JAP 110, 074508 (2011).

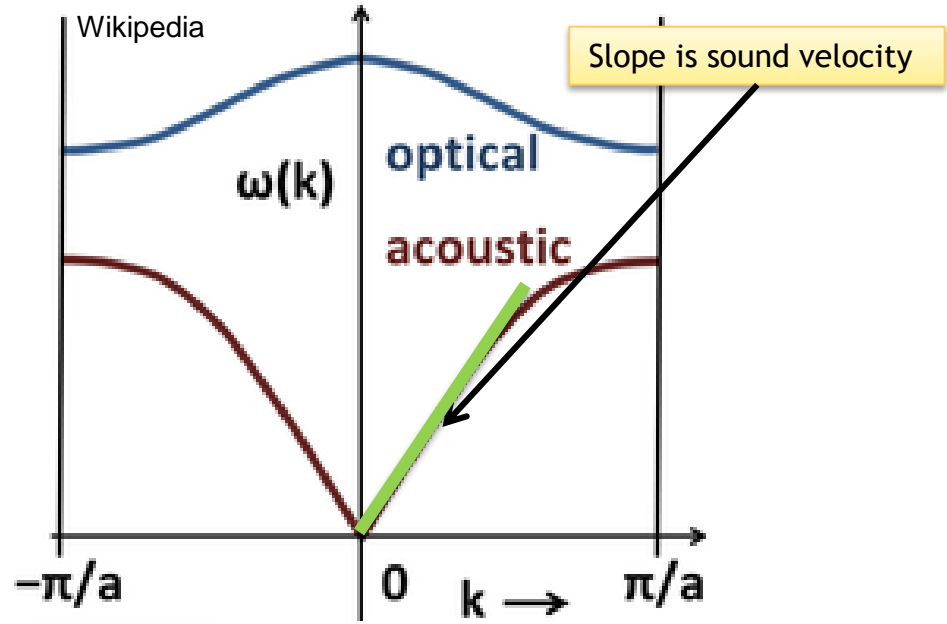


(1) and (2) can only be covered with scattering

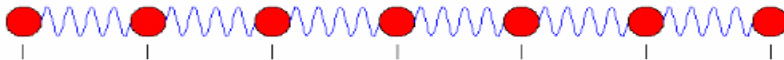
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- With bulk phonons, the perturbing potential (electron-phonon interaction strength) is solved analytically
- Assume:
  - linear dispersion
  - bulk phonons in equilibrium
  - elastic
  - high temperature



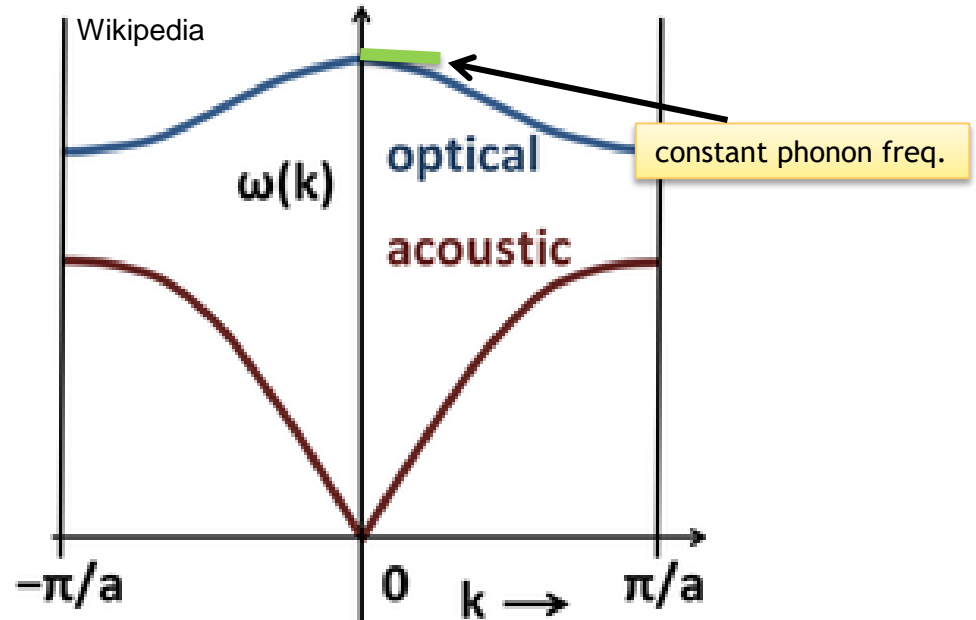
long wavelength acoustic phonon



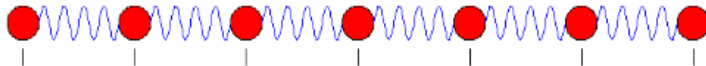
Scattering Parameters:

- ion mass density
- sound velocity
- deformation potential

- With bulk phonons, the perturbing potential (electron-phonon interaction strength) is solved analytically
- Assume:
  - flat dispersion
  - bulk phonons in equilibrium
  - inelastic



Optical phonon



### Scattering Parameters:

- ion mass density
- phonon frequency
- optical deformation constant

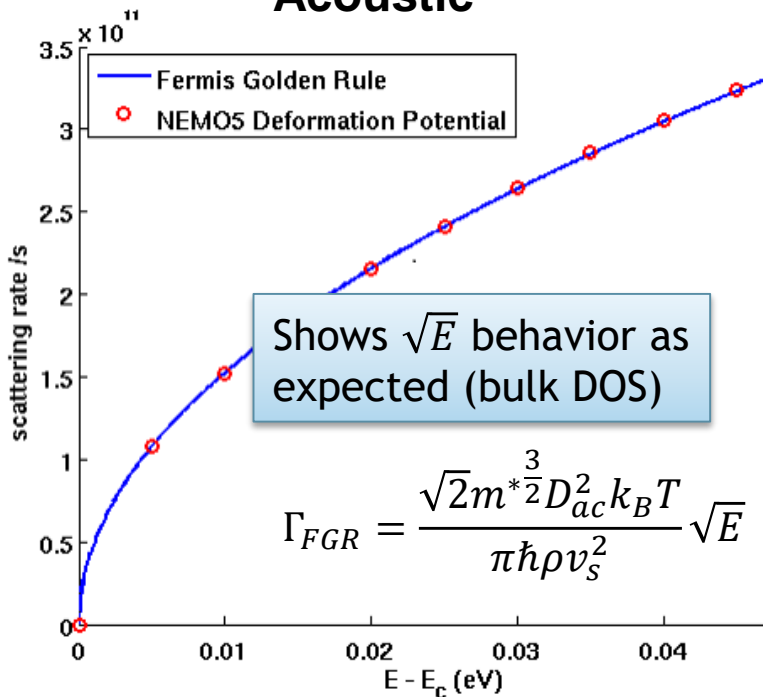
Both can be verified against analytical expressions for scattering rate

$$\Gamma_{NEGF}(E) = -\frac{2}{\hbar} \text{Im}\{\Sigma_{\text{scatt}}^R(E)\}$$

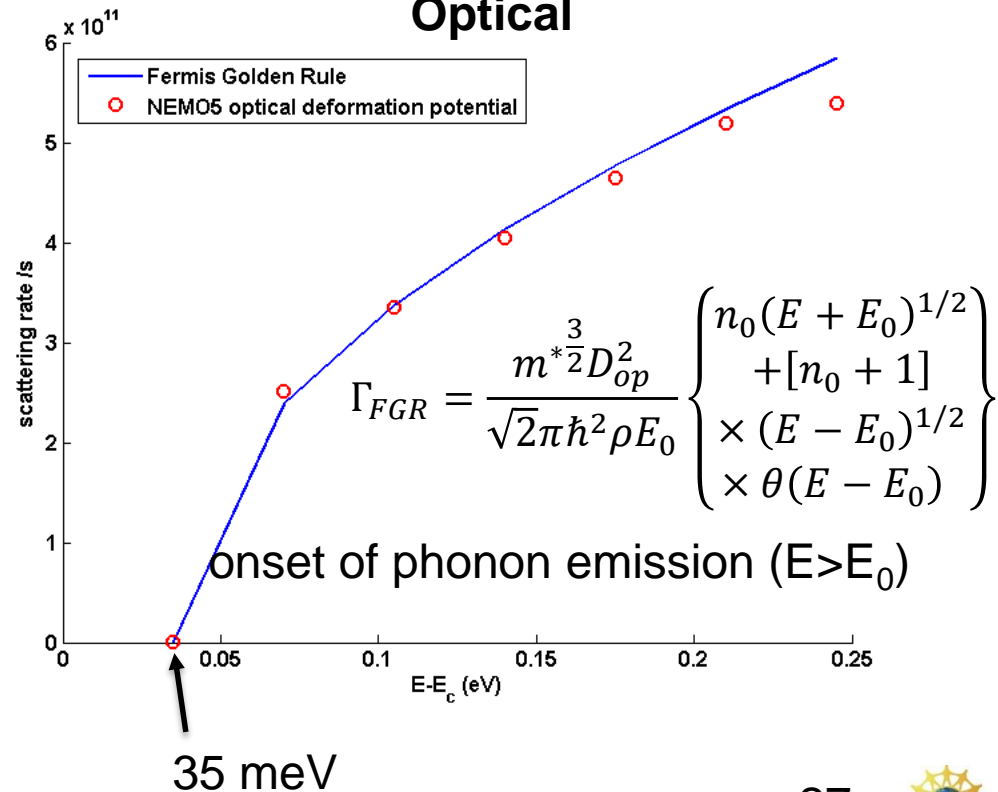
Bulk GaAs Material Parameters\*:

- Deformation potential  $D_{ac} = 8.8$
- Sound velocity  $v_s = 4726$  m/s
- Material density  $\rho = 5317$  kg/m<sup>3</sup>
- Phonon energy  $E_0 = 35$  meV
- Optical Coupling constant  $D_{op} = 110$  eV/nm

### Acoustic



### Optical

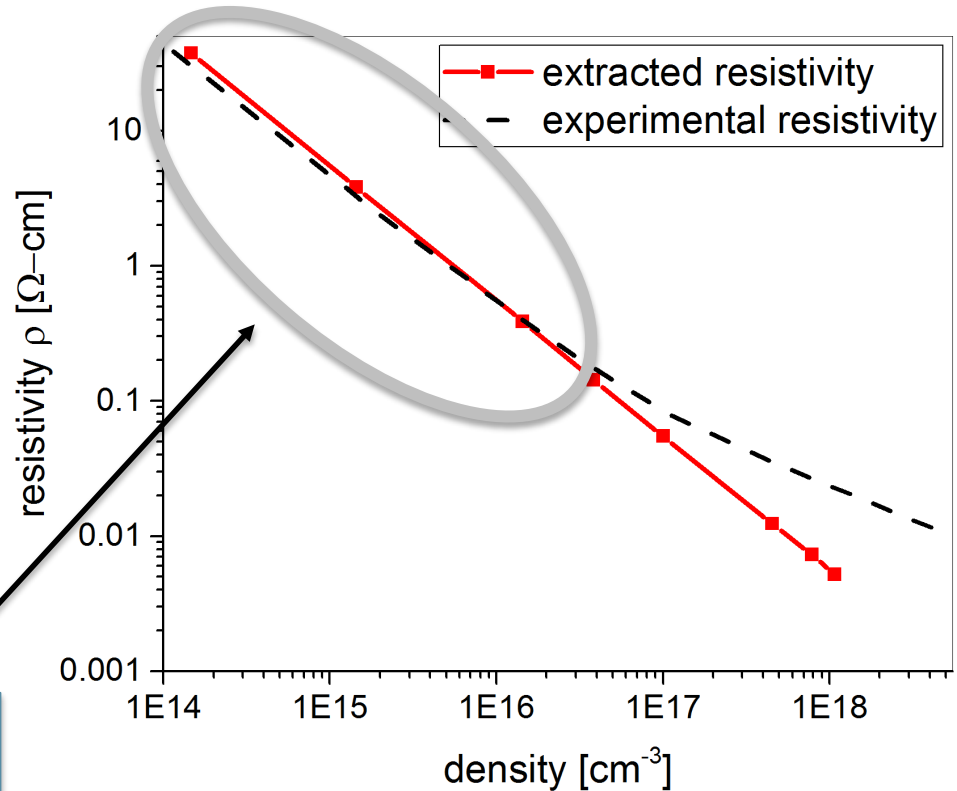


Device: homogeneous silicon bar in effective mass

Steps:

1. Calculate current of different lengths with small applied potential (5 meV)
2. Calculate slope of resistance vs. length

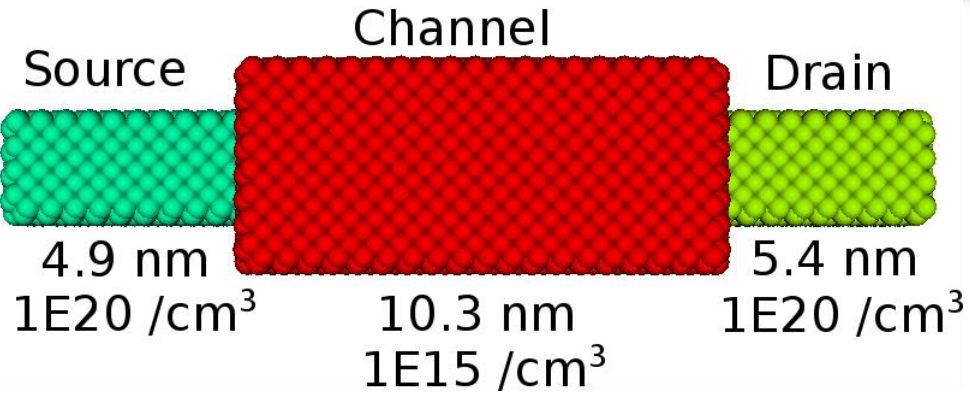
Deviation due to neglect of electron-electron and impurity scattering



Matches well for phonon-limited range

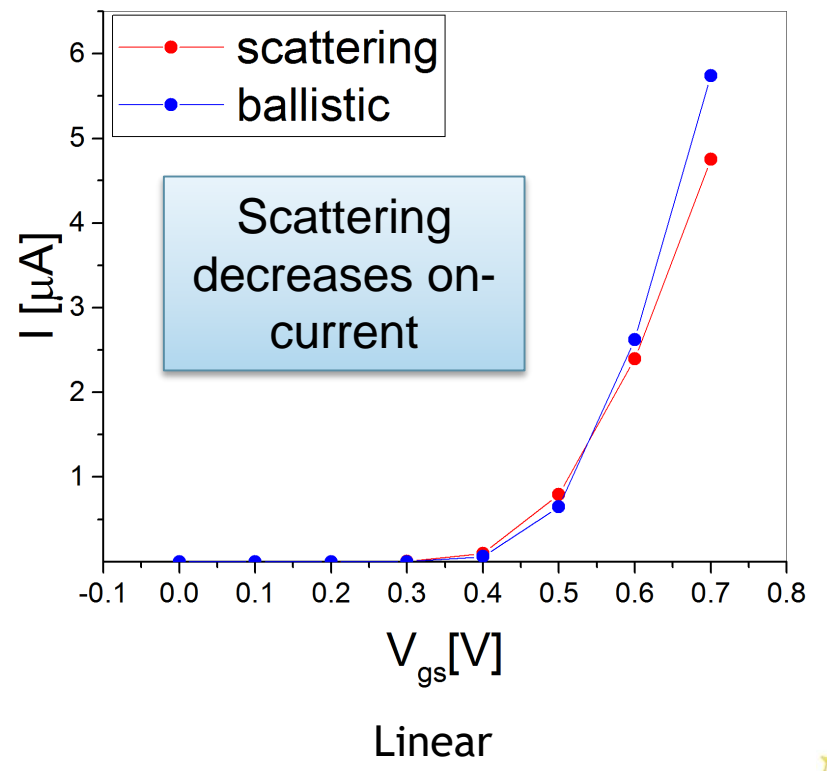
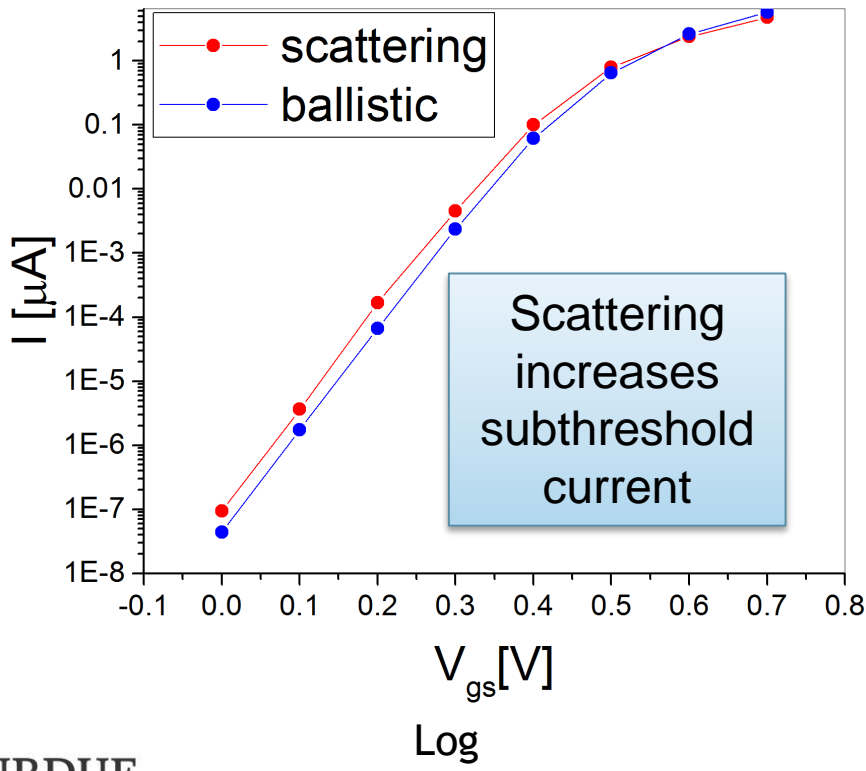
Experimental data from NIST

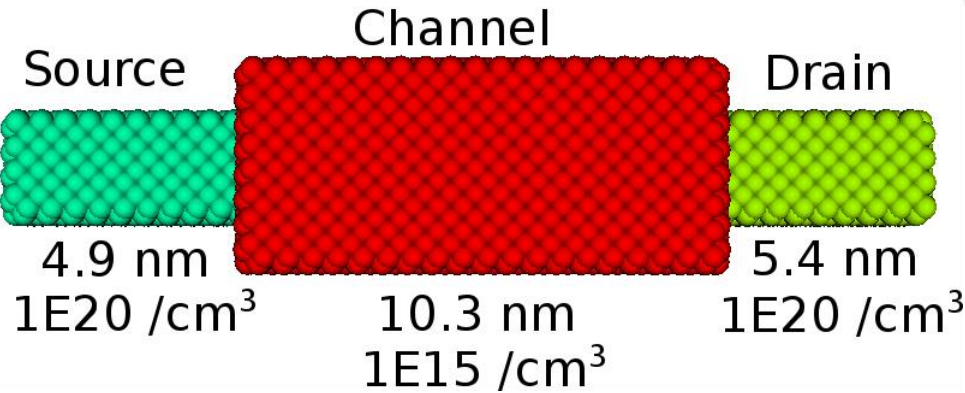
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Si, 2nm cross section  $sp^3d^5s^*$

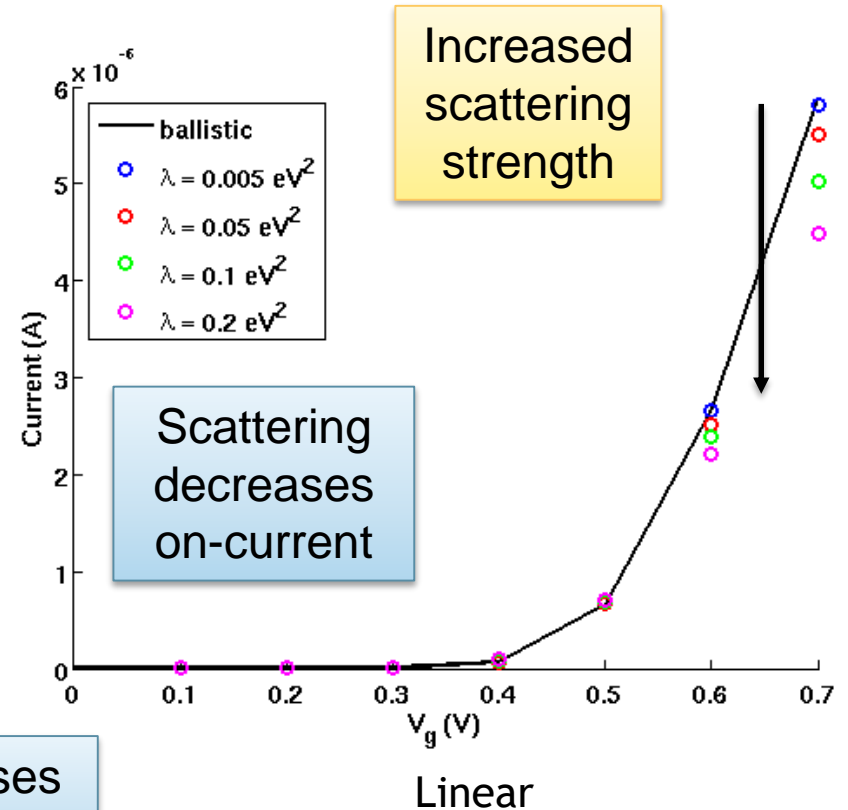
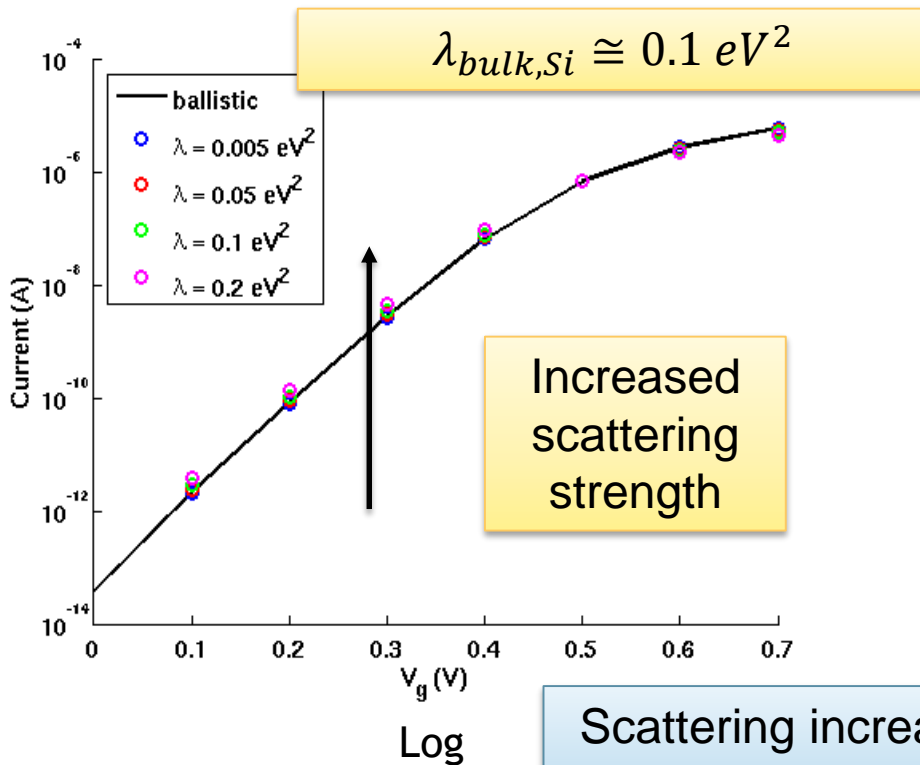
NIN nanowire elastic  
acoustic + optical





Si, 2nm cross section  $sp^3d^5s^*$   
 NIN nanowire elastic acoustic

$$\lambda = \frac{k_B T D_{ac}^2}{\hbar v_s^2 \rho} \delta_{\alpha}$$



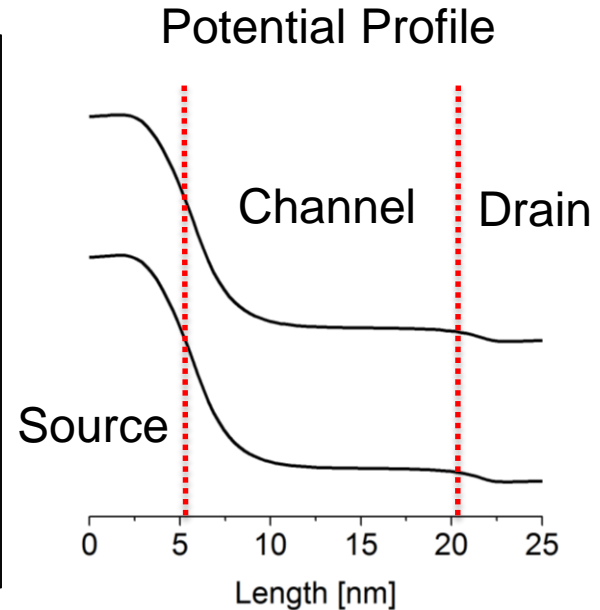
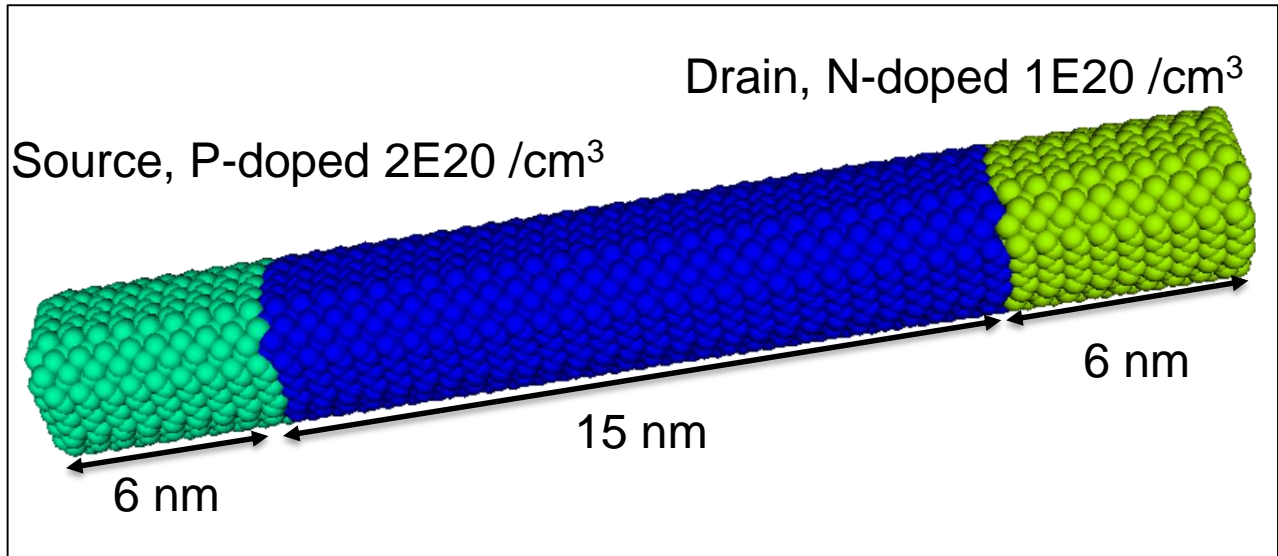
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**Question:**

What is the impact of scattering on TFETs?

**Circular Si TFET 3nm cross section**



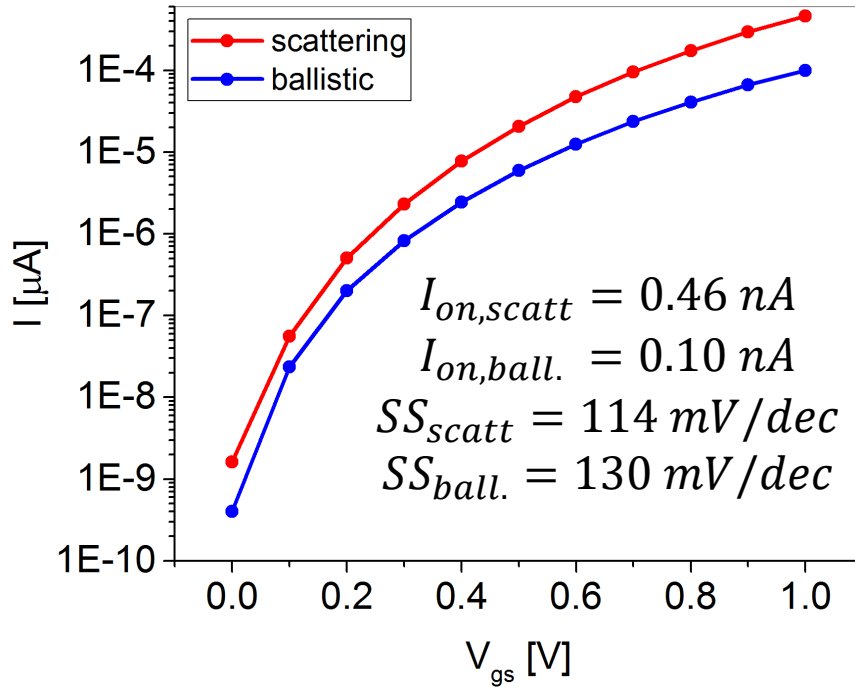
1nm thick oxide covers entire device (not shown)

$$V_{ds} = 1.0V$$

**Deformation potential phonons included:**

Elastic acoustic and inelastic optical phonon self-energies

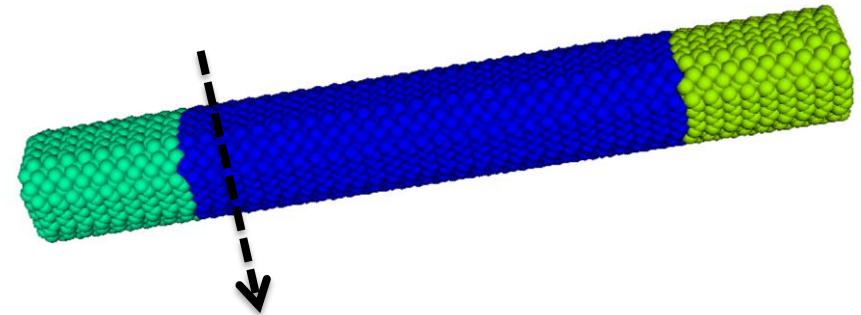
### TFET IV characteristics



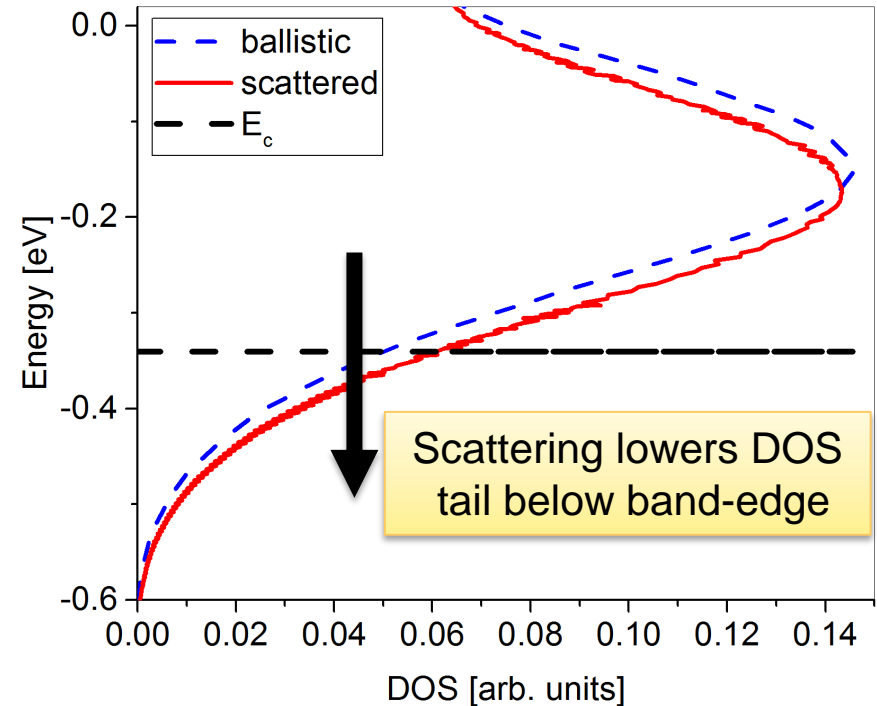
Impact of incoherent scattering:

- Increase and shift of band tails
- Increase of tunneling current by ~4x

Realistic TFET performance prediction questionable without scattering



Density of states along cut



### Question:

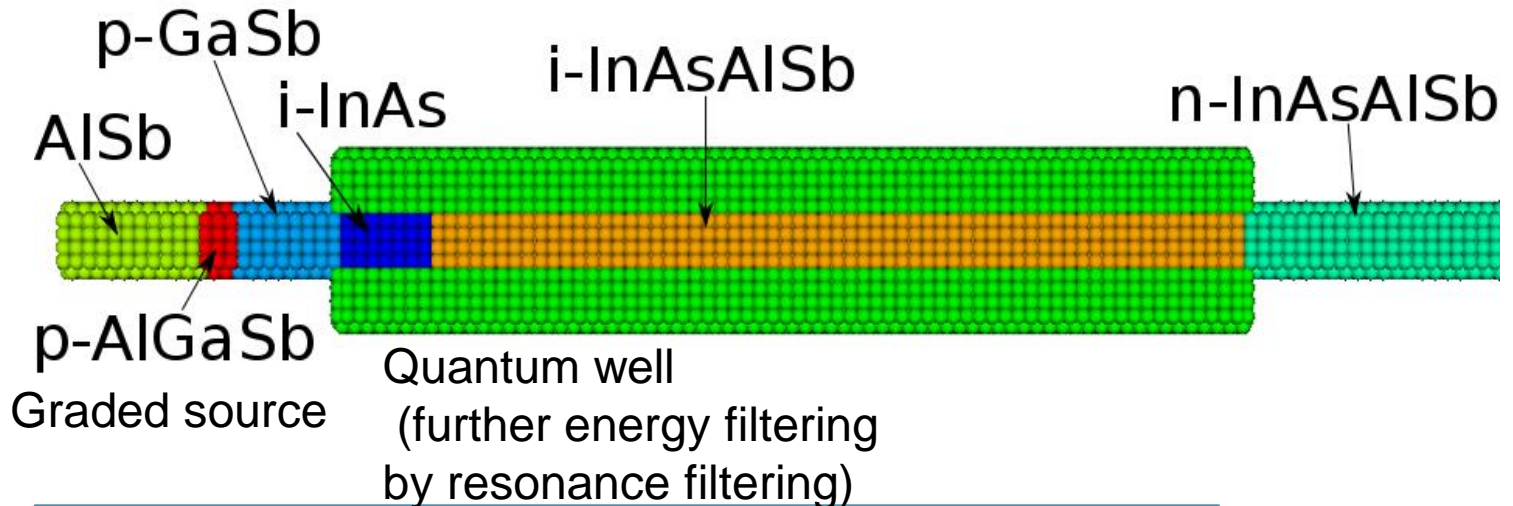
What is the impact of scattering on a III-V resonant TFET?

Dominant scattering in III-Vs is polar optical phonon (POP) scattering

### Assumptions:

Treat POP scattering as diagonal (non-polar optical) with increased scattering strength. Why? It is numerically feasible but loses nonlocality information.

TFET design by Pengyu Long, et. al. DRC (2016).

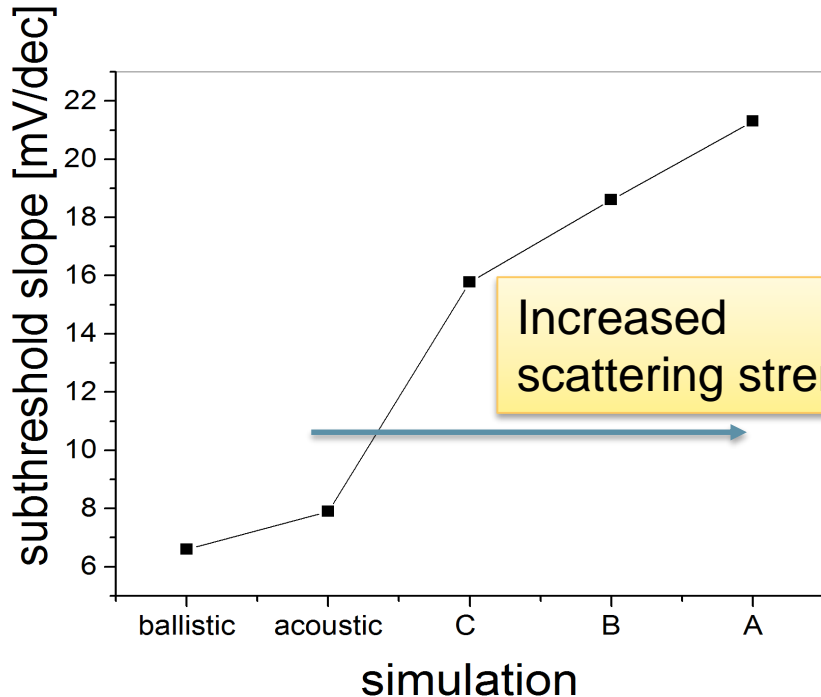
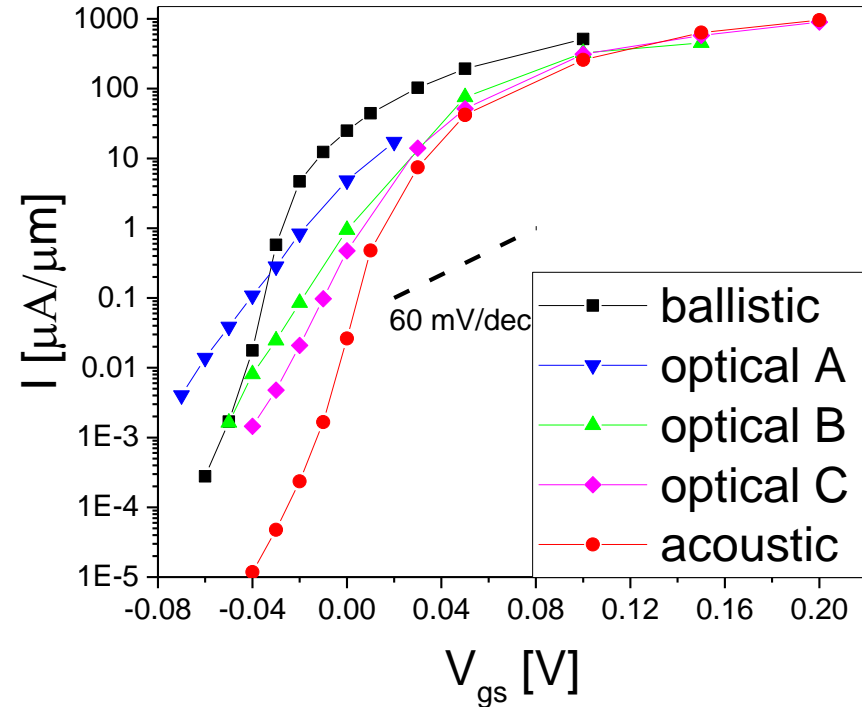


Scattering used to help assess design feasibility

Optical phonon energy 35 meV

Simulations ran by Devin Verrick

	Strength
ballistic	
Optical A	Optical C * 4
Optical B	Optical C * 1.85
Optical C	Si non-polar def. const.
acoustic	Bulk GaAs parameters

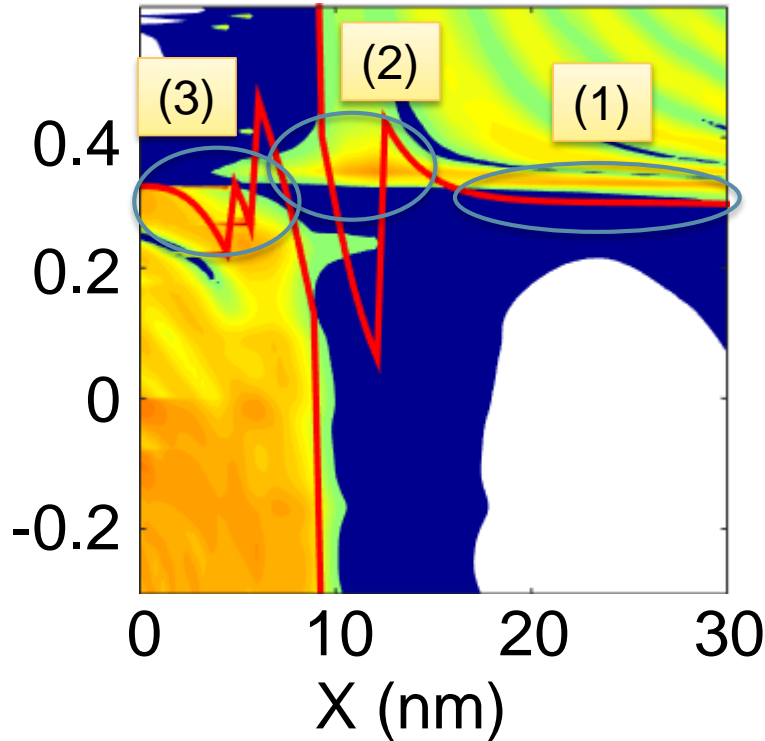


Scattering degrades subthreshold slope

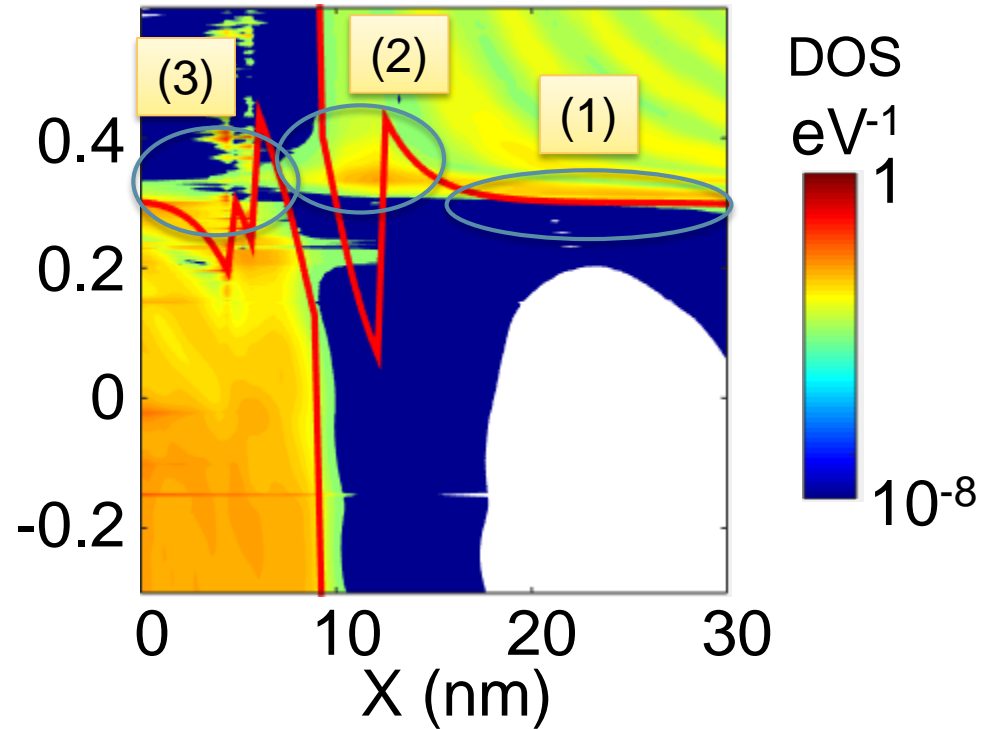
Similar to ballistic – scattering weak

Simulations and figures by Devin Verrick

Acoustic



Acoustic + NPO 220eV/nm



Inelastic scattering increases:

- (1) Tunneling below band edge
- (2) Penetration of resonance state into bandgap
- (3) Coupling of source hole states to resonance states

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Approximation I: Neglect  $Re\{\Sigma^R\}$  completely. Solve  $\Sigma^>$  and  $\Sigma^<$   
 $\Sigma^R \cong \frac{1}{2}(\Sigma^> - \Sigma^<)$  then neglecting the principal value integral.

broadening only

Approximation II: Keep part of  $Re\{\Sigma^R\}$  by solving  $\Sigma^R$  and  $\Sigma^<$  then neglecting the (partial) principal value integral.

broadening + part of energy shift

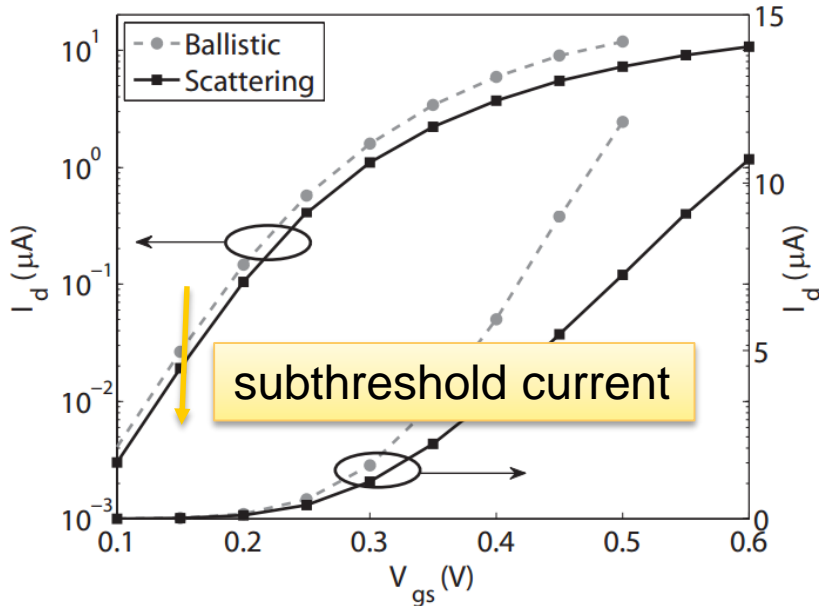
Full: Solve principal value integral

broadening + energy shift

Using Approximation II is a compromise between efficiency and accuracy

### Approximation I

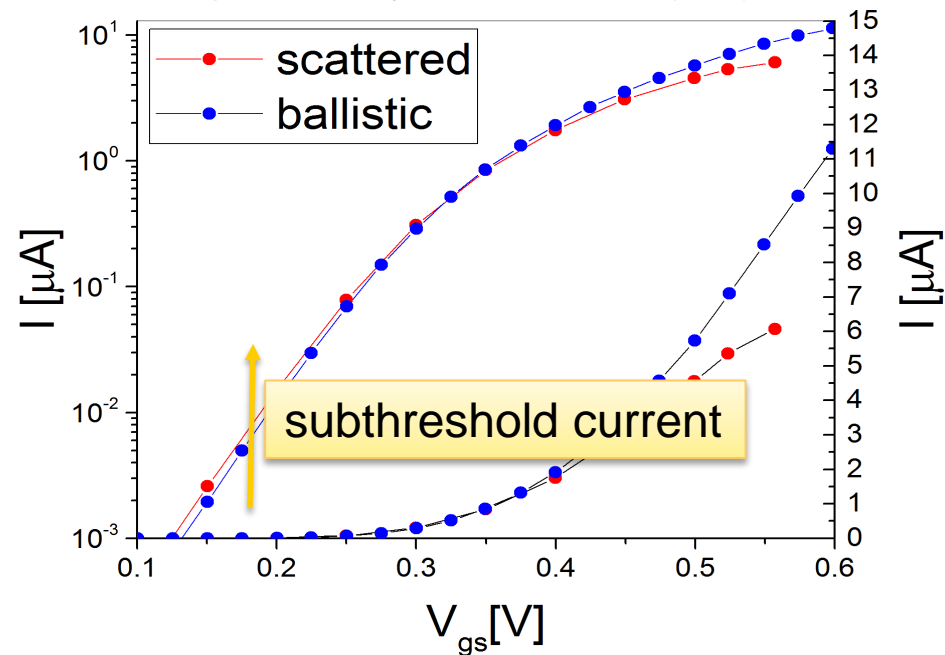
M. Luisier and G. Klimeck Phys. Rev. B **80**, 155430 (2009).



3 nm circular silicon nanowire,  $V_{ds} = 0.6\text{V}$   
 $sp^3d^5s^*$  tight binding basis  
 confined phonon model

### Approximation II

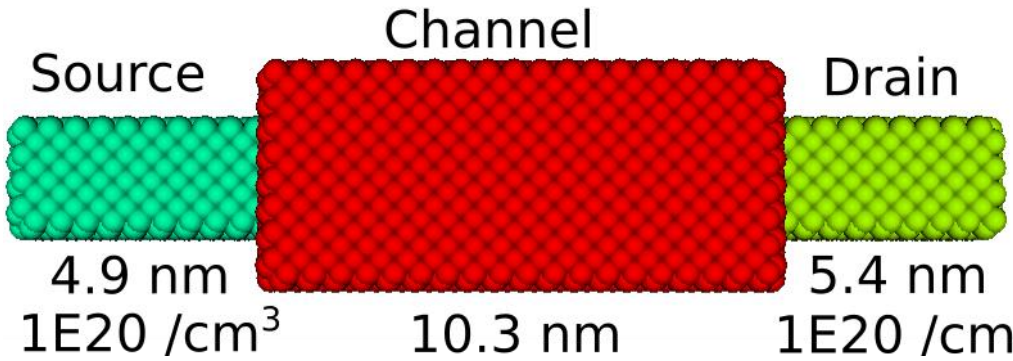
Data from A. Esposito, M. Frey, et. al. JCEL vol. 8 (2009).



3.2 nm square silicon nanowire,  $V_{ds} = 0.5\text{V}$   
 non-parabolic effective mass basis  
 bulk phonon model

Maybe the difference in approximations made lead to conflicting trends?

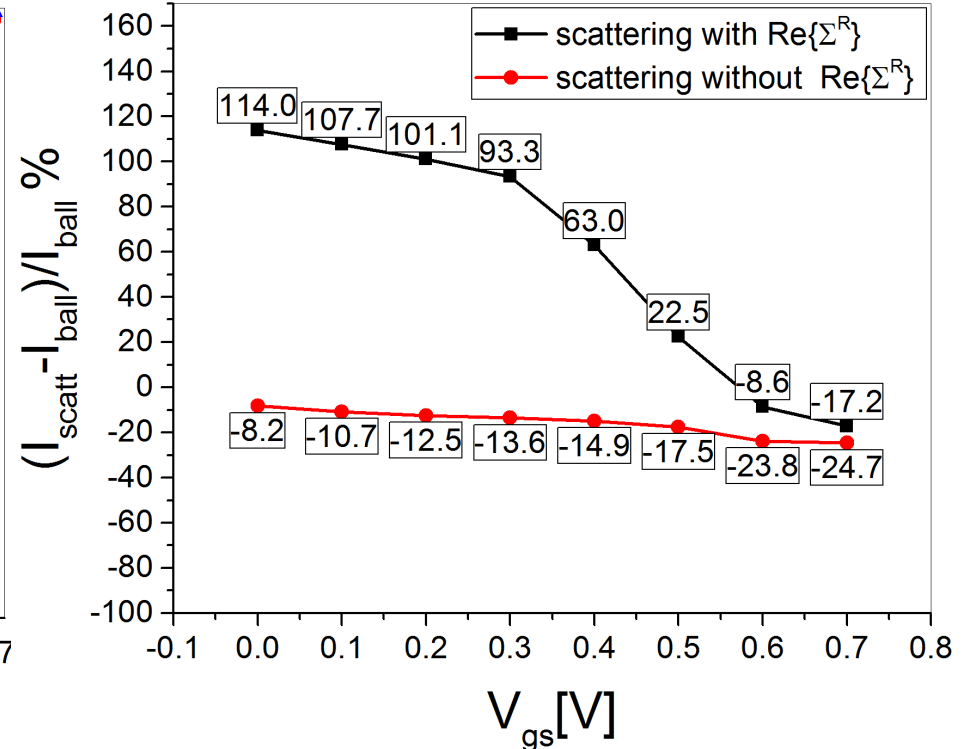
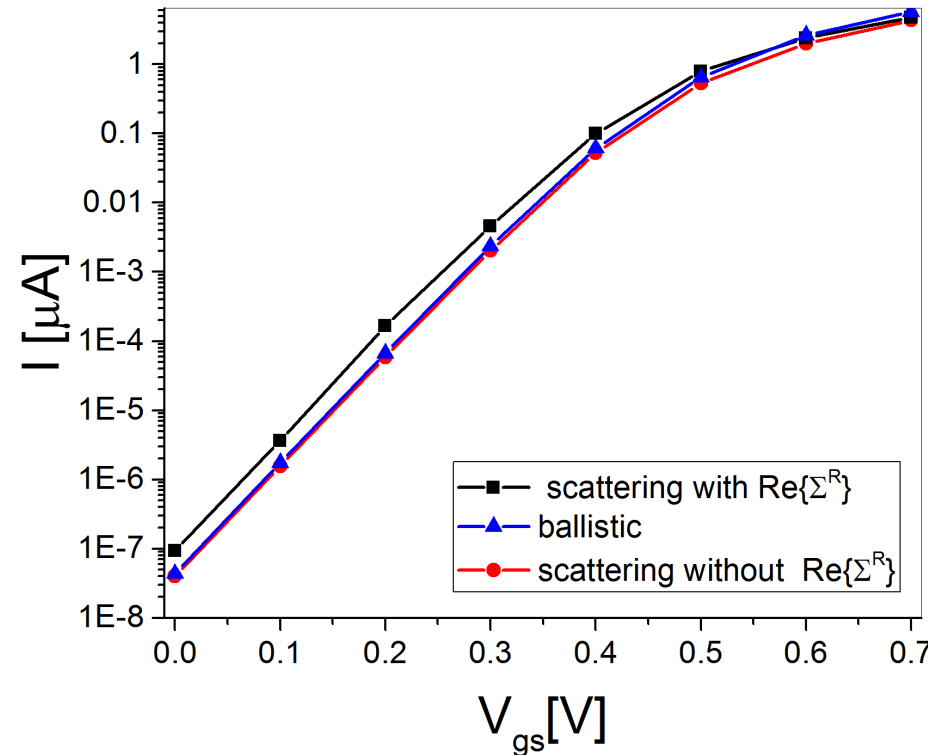




Si, 2nm cross section  $sp^3d^5^*$

NIN nanowire

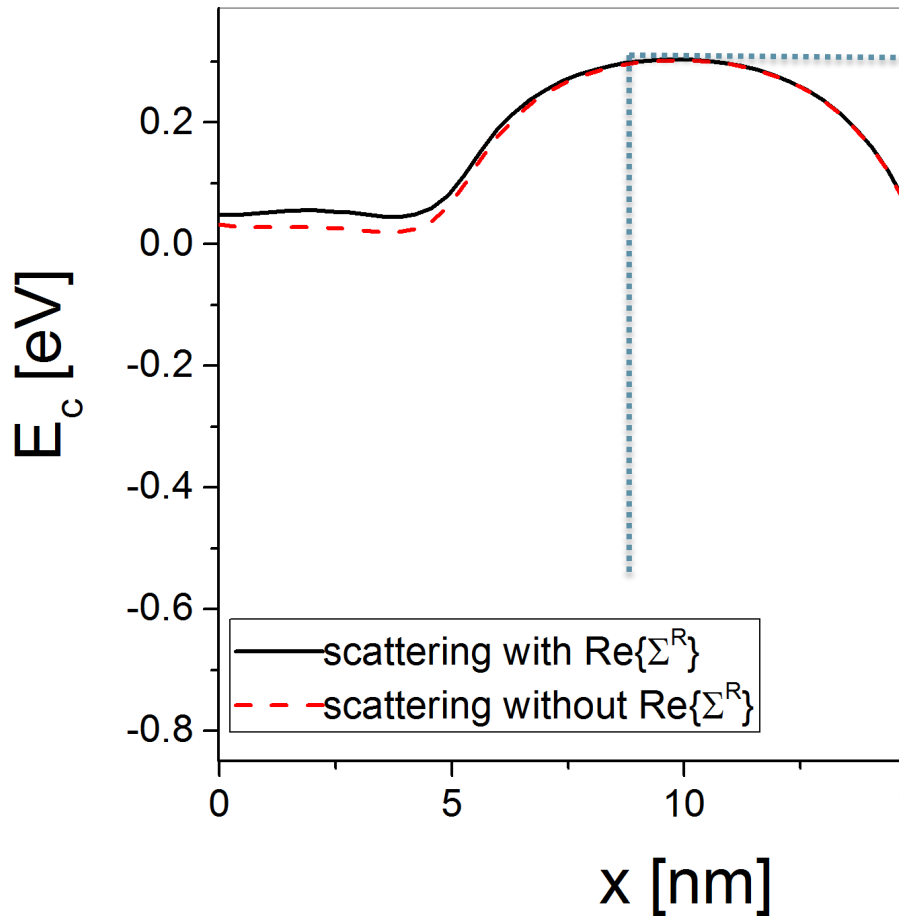
Relative Error  $(I_{scatt} - I_{ball})/I_{ball}$



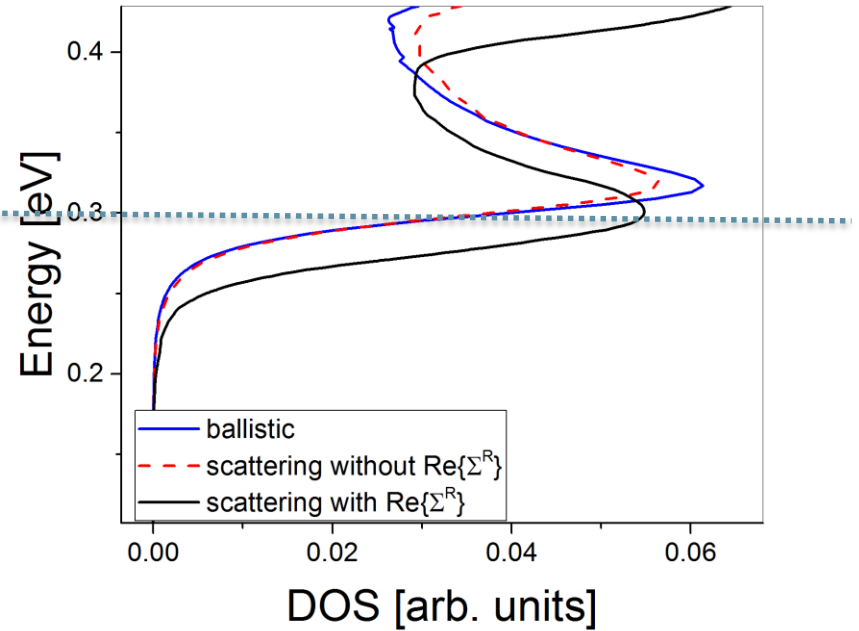
Neglecting  $Re\{\Sigma^R\}$  (Approximation I) underestimates subthreshold current

$V_{gs}=0.2V, V_{ds}=0.8V$

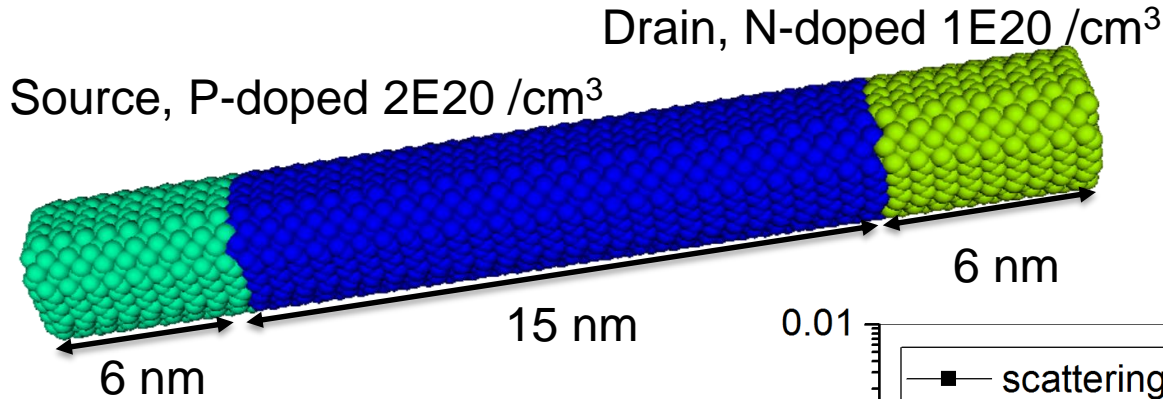
1D conduction band edge through center of device



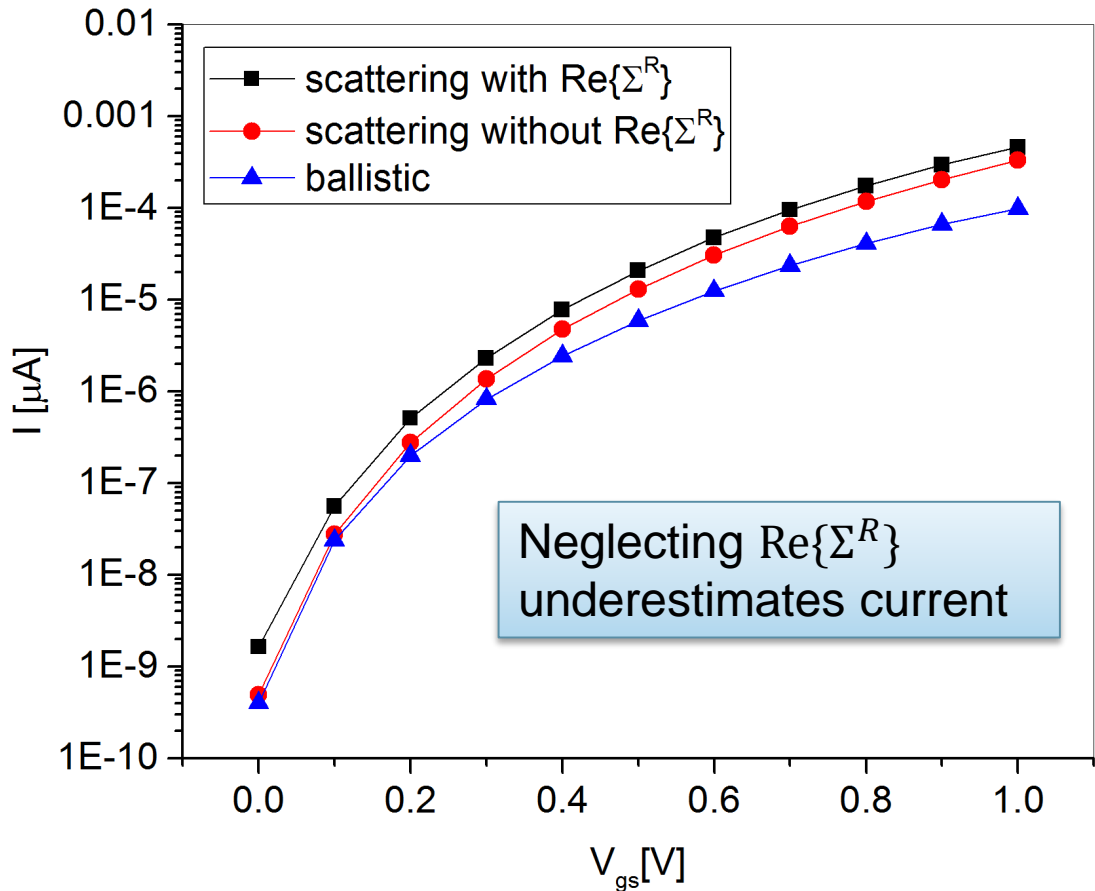
DOS lowered beneath band edge



$\frac{3}{4}$  Peak – Full Maximum  
 Ballistic 38 meV  
 With  $Re\{\Sigma^R\}$  50 meV  
 Without  $Re\{\Sigma^R\}$  45 meV



Si, 3nm diameter  $sp^3d^5s^*$   
PIN nanowire TFET



- 1) Motivation
- 2) Acoustic and Optical Phonon Scattering Verification
- 3) Effect of scattering on MOSFETs
- 4) Effect of scattering on TFETs
- 5) Why does scattering increase tunneling current?
- 6) Numerical Details**
- 7) Conclusions/Future Work

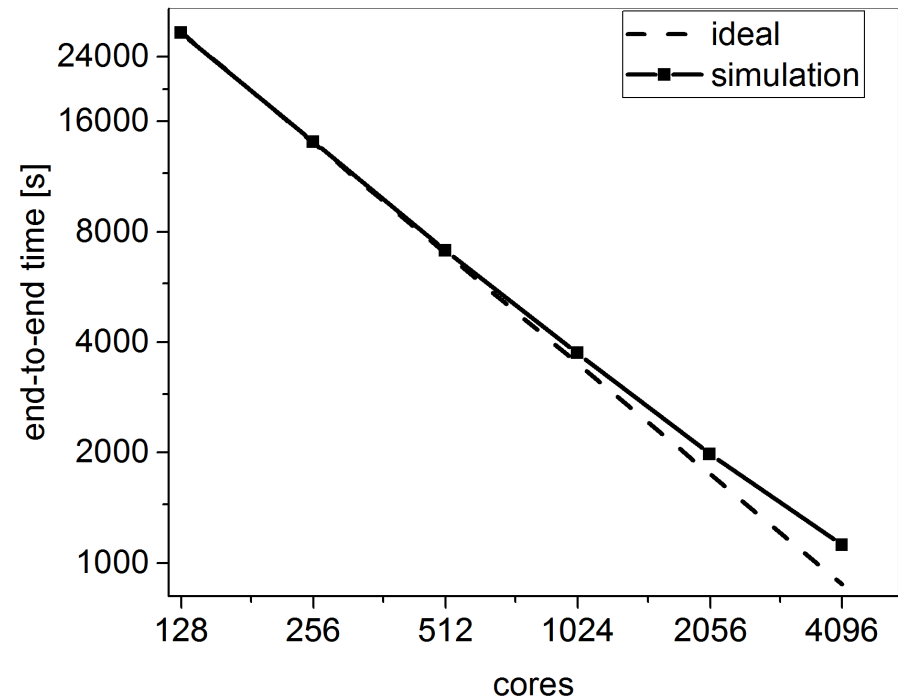
Scattering self-energies requires energies that can be on different MPI processes:

$$\Sigma^<(E) = \frac{\hbar}{2\rho\omega_o} \delta(\vec{x}_3 - \vec{x}_4) [N_{op}G^<(E - E_{op}) + (N_{op} + 1)G^<(E + E_{op})]$$

Requires communication of diagonal matrices

Note: for UTB simulations there is an additional wave-vector  $k$  integral that increases communication

Device: Si TFET used for IV



Reasonable scaling despite complex communication

- Stabilized Recursive Green's Function algorithm
- Improved Poisson convergence with improved Jacobian
- Interpolated scattering self-energies to decrease number of scattering iterations needed and improve current conservation
- Implemented dynamical convergence to decrease number of scattering iterations needed
- Current conservation in optical phonon scattering with inhomogeneous energy grid
- Improved resonance mesh suitable for resonant devices

## Objective:

Efficient implementation of recursive Green's function (RGF) algorithm suitable for scattering

## Problem:

Initial implementation of RGF in NEMO5 following OMEN was unstable when scattering was included.

## Approach:

- Systematic analysis of RGF equations to find source of instability.
- Remove assumptions of symmetries only valid with infinite precision
- Preserve symmetry of equations in each recursive iteration

## Results/Impact:

Found instabilities and improved RGF algorithm to allow scattering simulations.

Before:

$$G_{i,i}^< = g_{i,i}^< + g_{i,i}^R H_{i,i+1} G_{i+1,i+1}^< H_{i+1,i} g_{i,i}^A + g_{i,i}^R H_{i,i+1} G_{i+1,i+1}^R H_{i+1,i} g_{i,i}^< - (g_{i,i}^R H_{i,i+1} G_{i+1,i+1}^R H_{i+1,i} g_{i,i}^<)^{\dagger}$$

After:

$$G_{i,i}^< = g_{i,i}^< + g_{i,i}^R H_{i,i+1} G_{i+1,i+1}^< H_{i+1,i} g_{i,i}^A + g_{i,i}^R H_{i,i+1} G_{i+1,i+1}^R H_{i+1,i} g_{i,i}^< + (g_{i,i}^R H_{i,i+1} G_{i+1,i+1}^R H_{i+1,i} (g_{i,i}^<)^{\dagger})^{\dagger}$$

Additionally:  $G_{i,i}^<$  is anti-symmetrized each iteration.

### Objective:

Convergence of NEGF-Poisson equations with minimum number of iterations

### Problem:

Ballistic Jacobian typically used in NEMO5 is not suitable for scattering

### Approach:

- Balance between number of iterations needed and calculation time of Jacobian
- Found best balance is to use a mixture of ballistic Jacobian (extra NEGF solution) and approximate scattering Jacobian

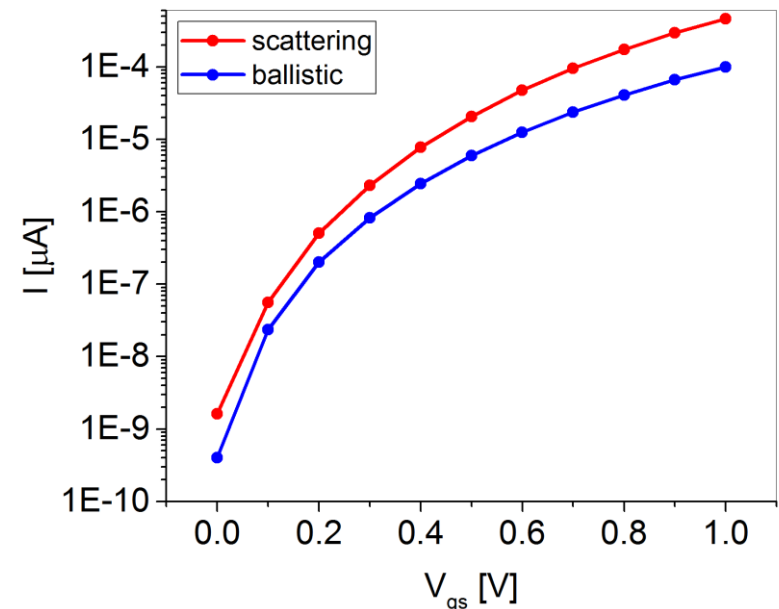
### Results/Impact:

Convergence achieved for previously not converging simulations.

Jacobian where  $\lambda$  is a mixing parameter

$$J(\vec{x}) = \mathfrak{I} \left\{ \lambda \int G_{ballistic}^<(\vec{x}, E, \frac{\partial f_{S,D}}{\partial E}) dE + \int (1 - \lambda) G_{scattered}^<(\vec{x}, E, f_{S,D}) dE \right\}$$

Si circular nanowire TFET





### Objective:

Minimum number of self-consistent Born approximation (SCBA) iterations to reach converged result

### Problem:

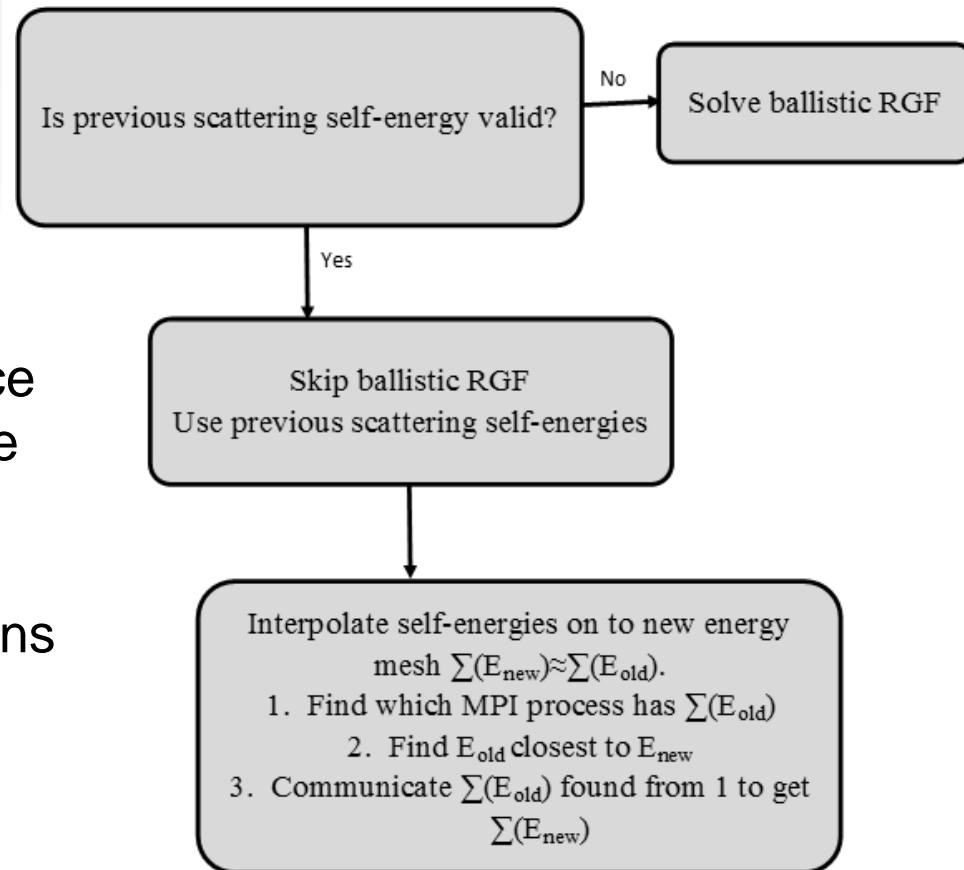
Typically for current conservation, self-consistent Born needs 20-40 computationally expensive iterations

### Results/Impact:

- Discovered that when Poisson-NEGF loop is close to convergence previously scattered results can be interpolated on to the updated energy mesh
- Reduced number of SCBA iterations by about 3

### Approach:

- Reuse previously converged SCBA results to accelerate convergence of updated Poisson potentials



## Objective:

Minimum number of self-consistent Born approximation (SCBA) iterations to reach converged result.

## Problem:

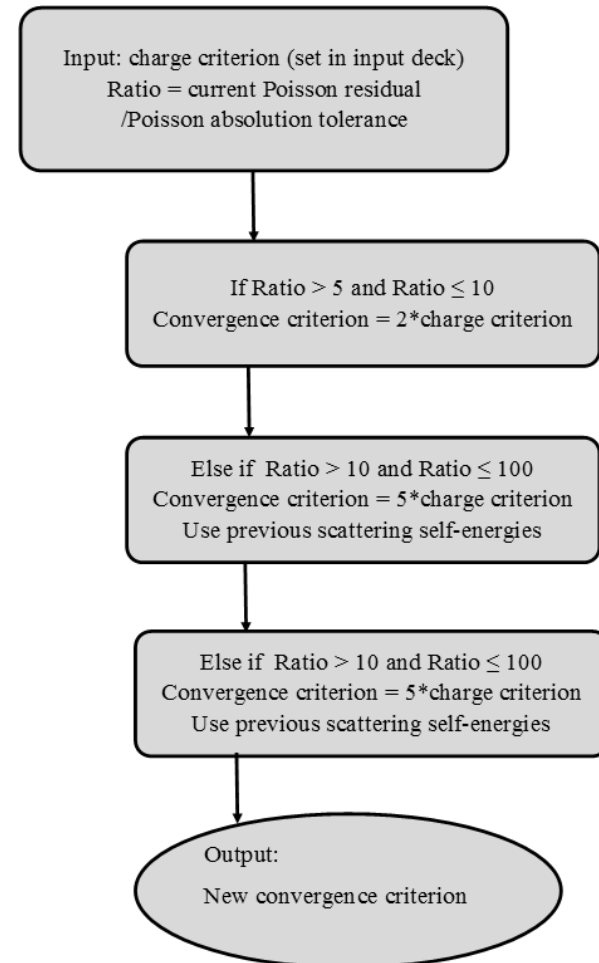
Typically for current conservation, self-consistent Born needs 20-40 computationally expensive iterations

## Results/Impact:

Reduced number of SCBA iterations by approximately half

## Approach:

- Reduce the number of SCBA iterations without making additional approximations



### Objective:

Current conservation criterion for converged self-consistent Born results

### Problem:

For efficient simulations, an inhomogeneous energy mesh must be used but the energy mesh will not be commensurate with phonon energies, thus current conservation is not trivial.

### Approach:

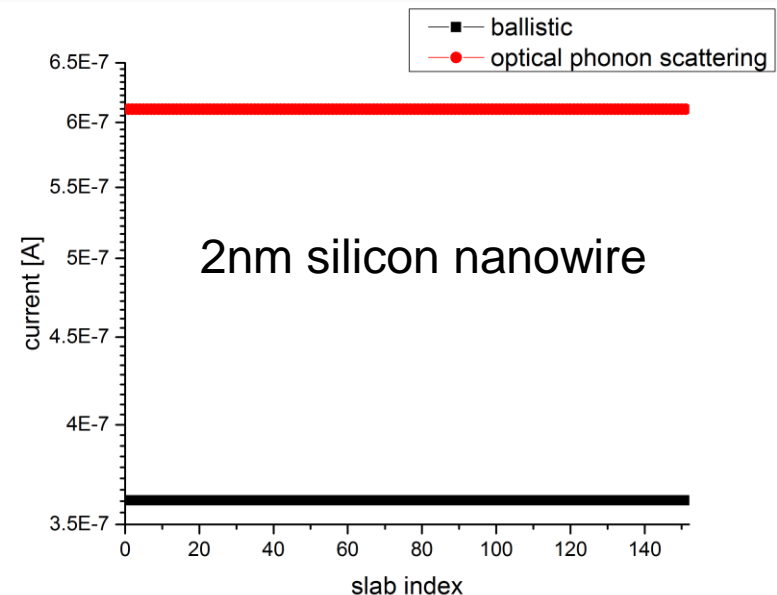
- Ensure detailed balance is always met and use this constraint to form constraints on interpretation of scattering self-energies

$$\int (\Sigma^<(E)G^>(E) - G^<(E)\Sigma^>(E))dE = 0$$

“in-scattering must balance out-scattering”

### Results/Impact:

Current Conservation with general energy mesh



### Objective:

Convergence of NEGF-Poisson equations with minimum number of iterations

### Problem:

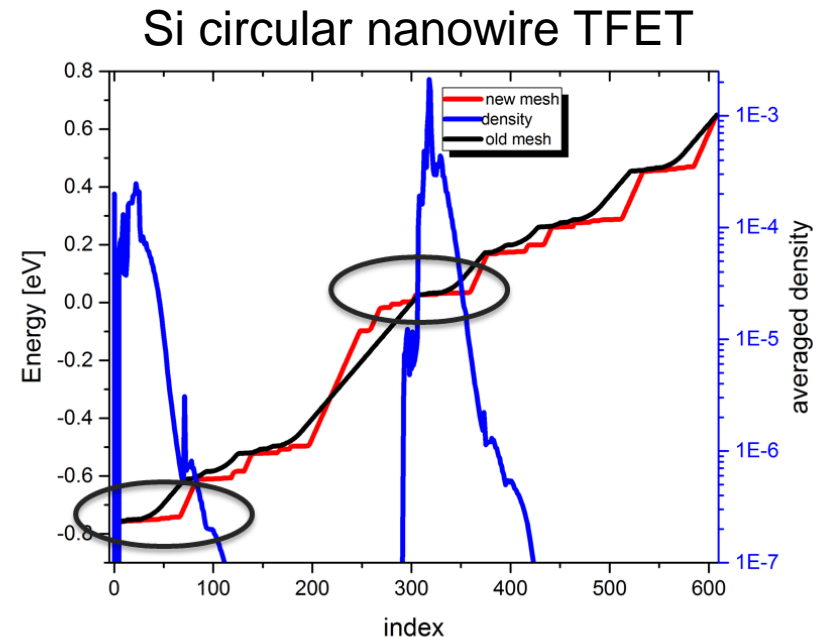
Scattering introduces resonance shifts that must be properly resolved

### Approach:

- Use device information in order to resolve resonances due to scattering
- Adapt energies to shifts in resonances

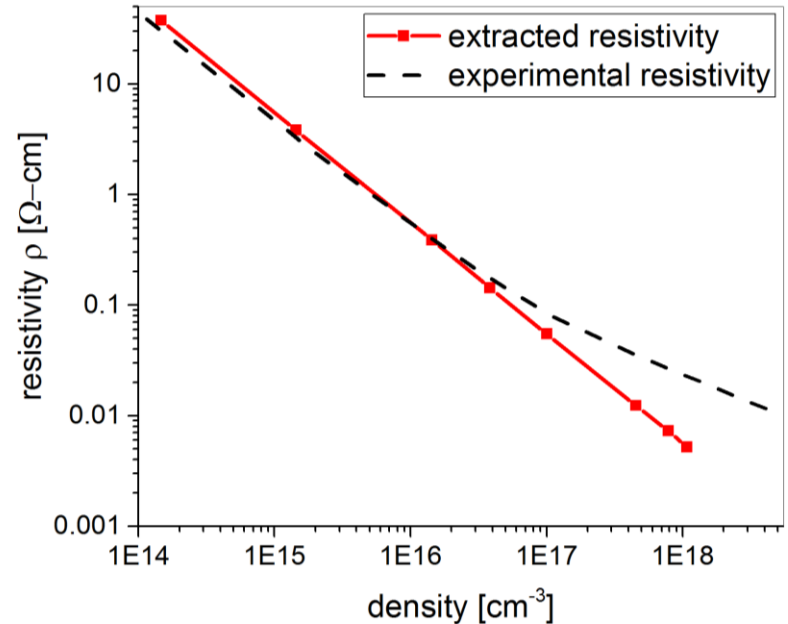
### Results/Impact:

- Improved convergence of NEGF-Poisson loop.
- Resonances due to scattering are properly resolved



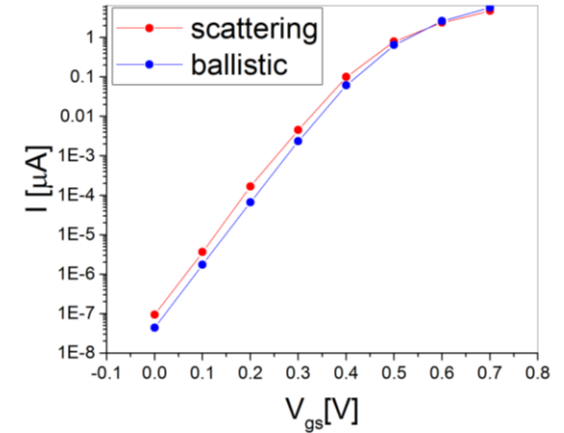
- 1) Motivation
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- 5) Why does scattering increase tunneling current?
- 6) **Conclusions/Future Work**

- Efficient implementation of scattering introduced
- Verification of implementation with comparison to Fermi's golden rule and to experimental resistivity

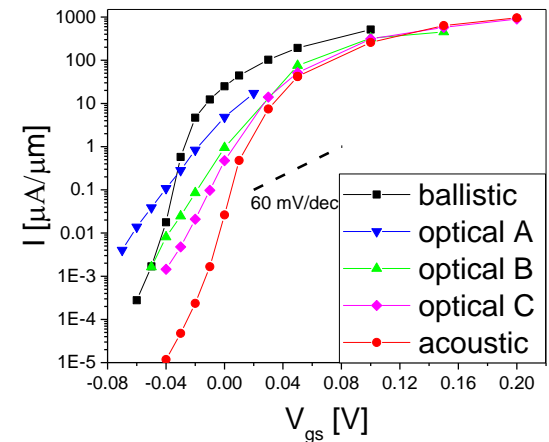
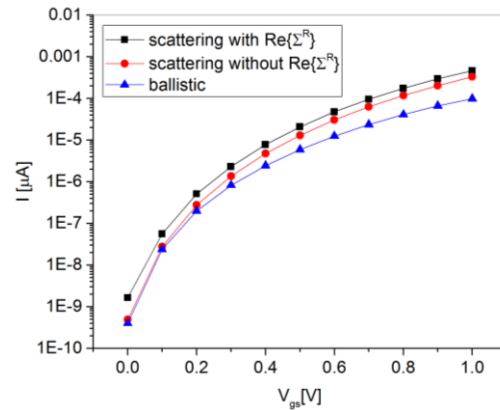


- Effect of certain approximations made in literature assessed

- MOSFET IV results with and without scattering



- TFET IV results with and without scattering compared



- Further assessment of approximations made e.g. local POP, bulk phonons.
- Comparison to heuristic models e.g. Klimeck's 1994 model "equilibrium-nonequilibrium" model
- Include other scattering mechanisms as scattering self-energies (e.g. roughness)
- Scattering model (phonons, roughness etc.) suitable for 2D materials e.g. TMDs



Thanks to:

my committee members: Professors Gerhard Klimeck, Supriyo Datta, Tillmann Kubis

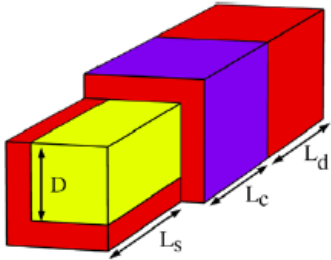
Administrative Staff

My groupmates and friends



# Questions?

## Backup Slides



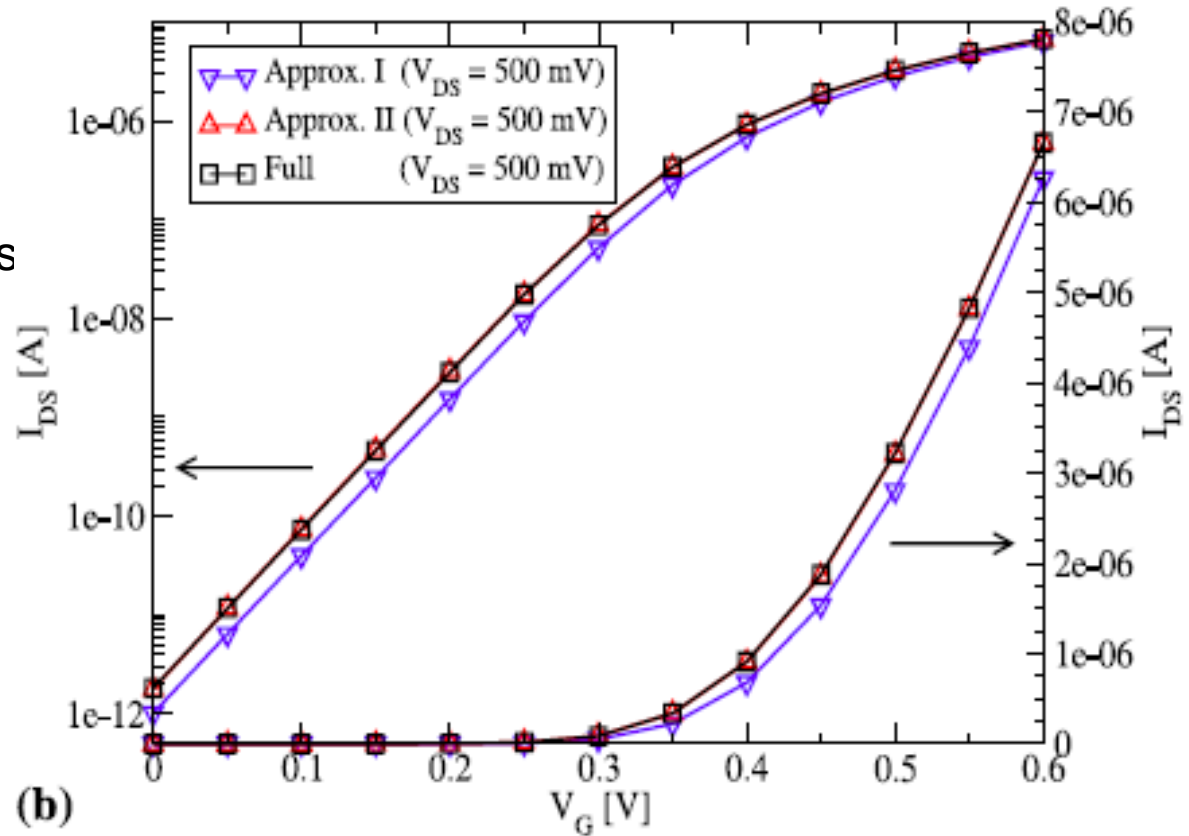
Si Nanowire in effective mass  
 $L_c = 15 \text{ nm}$ ,  $D = 3.26 \text{ nm}$

Approx. I –  $Re\{\Sigma^R\} = 0$

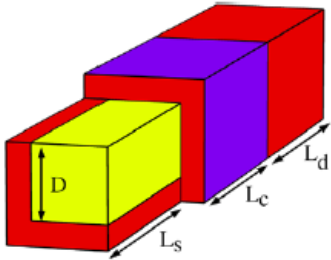
Approx. II –  $Re\{\Sigma^R\} \cong 0$

But neglect PVI

Full – includes PVI

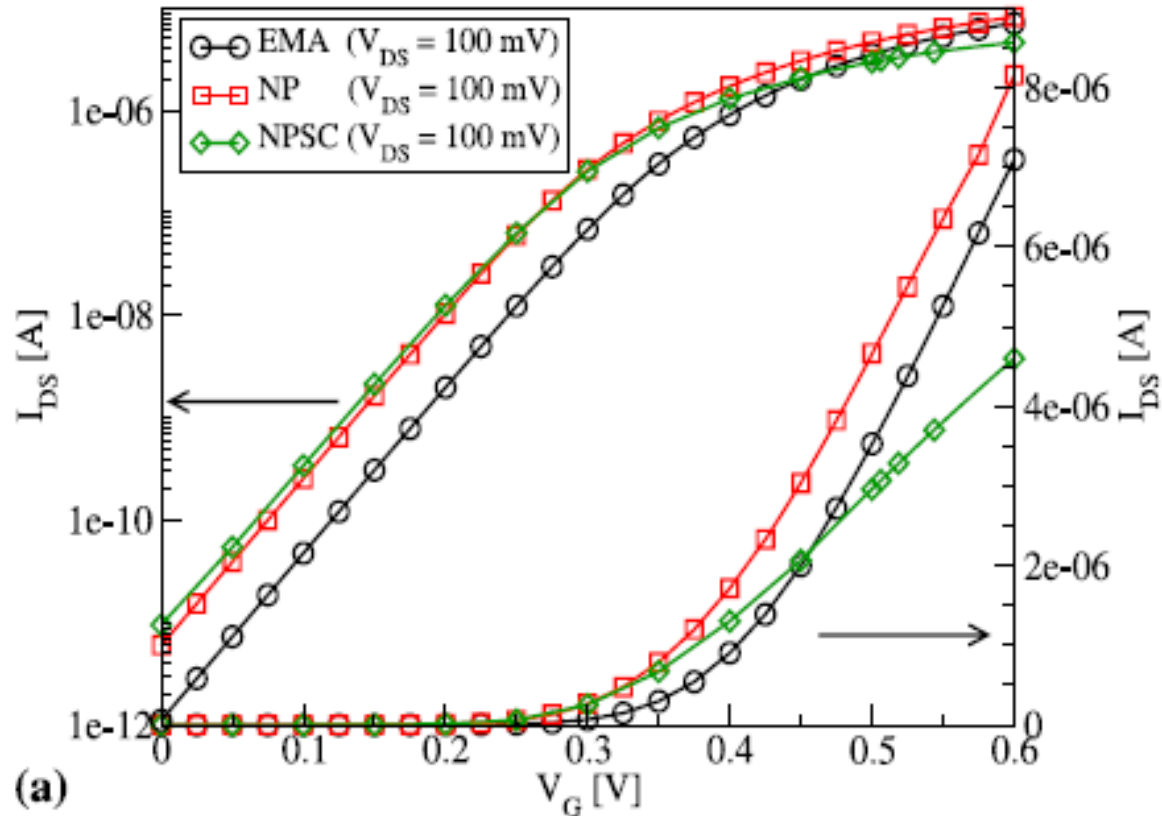


Neglecting  $Re\{\Sigma^R\}$  leads to underestimation of off-current.  
 NEMO5 uses Approx. II



Si Nanowire in effective mass  
 $L_c = 15 \text{ nm}$ ,  $D = 3.26 \text{ nm}$

NP – ballistic nonparabolic EM  
 NPSC –  
 Nonparabolic EM + Approx II  
 $Re\{\Sigma^R\} \cong 0$  But neglect PVI



Same trend as seen in NEMO5!

Esposito, Frey J. Comput Electron (2009).

$$\Sigma_{ac}^<(\alpha, \beta, E) = \frac{D^2 k_b T}{\rho v_s^2} \delta_{\alpha, \beta} G^<(\alpha, \beta, E)$$

\*"Quantum Transport in Semiconductor Nanostructures", T. Kubis PhD thesis (2009).

$N_{op}$  is independent of  $q$  (flat optical phonon band)

Long wavelength limit  $q \rightarrow 0$

Discrete energies for emission and absorption ( $E \pm E_{op}$ ) where  $E_{op} = \hbar\omega_o$

$$\Sigma^<(E) = \frac{\hbar}{2\rho\omega_o} \delta(\vec{x}_3 - \vec{x}_4) \left[ \begin{array}{c} \text{emission} \\ N_{op} G^<(E - E_{op}) + (N_{op} + 1) G^<(E + E_{op}) \end{array} \right]$$

$$\Sigma^R(E) = \frac{\hbar}{2\rho\omega_o} \delta(\vec{x}_3 - \vec{x}_4) \left[ N_{op} G^R(E + E_{op}) + (N_{op} + 1) G^<(E - E_{ac}) \right. \\ \left. + \frac{1}{2} G^<(E - E_{ac}) - \frac{1}{2} G^<(E + E_{ac}) \right]$$

Neglecting principal value integral

\*\*Quantum Transport in Semiconductor Nanostructures", T. Kubis PhD thesis (2009).

Approximation I:

$$\Sigma^R(E) = \frac{1}{2} (\Sigma^>(E) - \Sigma^<(E)) + iP \int \frac{dE'}{2\pi} \frac{(\Sigma^>(E') - \Sigma^<(E'))}{E - E'}$$

neglect

emission

absorption

Approximation II:

$$\Sigma^<(E) = \frac{\hbar}{2\rho\omega_o} \delta(\vec{x}_3 - \vec{x}_4) [N_{op} G^<(E - E_{op}) + (N_{op} + 1) G^<(E + E_{op})]$$

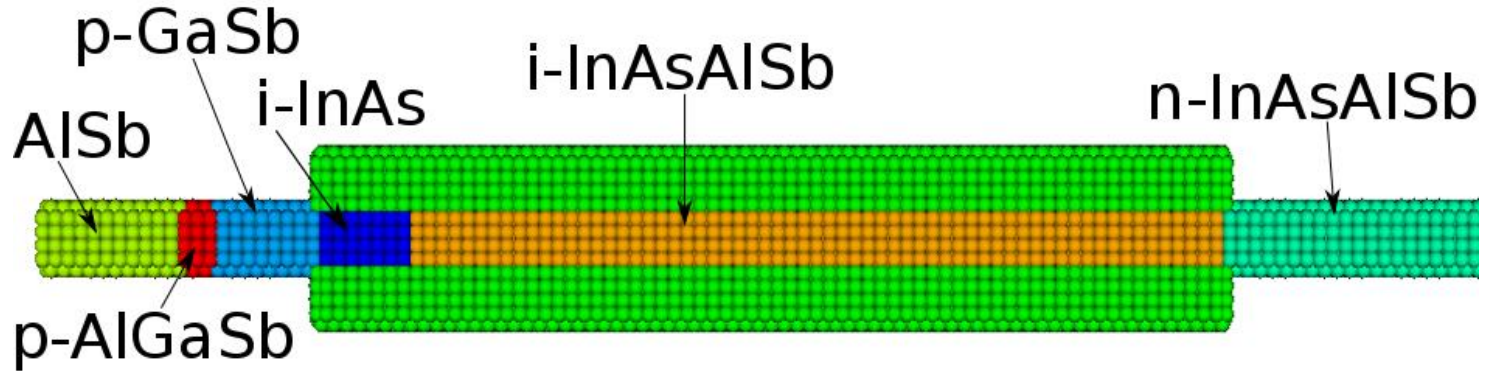
$$\Sigma^R(E) = \frac{\hbar}{2\rho\omega_o} \delta(\vec{x}_3 - \vec{x}_4) [N_{op} G^R(E + E_{op}) + (N_{op} + 1) G^<(E - E_{ac})$$

$$+ \frac{1}{2} G^<(E - E_{ac}) - \frac{1}{2} G^<(E + E_{ac})]$$

$$+ iP \int \frac{dE'}{2\pi} \left( \frac{G^<(E - E')}{E' - \hbar\omega_o} - \frac{G^<(E - E')}{E' - \hbar\omega_o} \right)$$

neglect

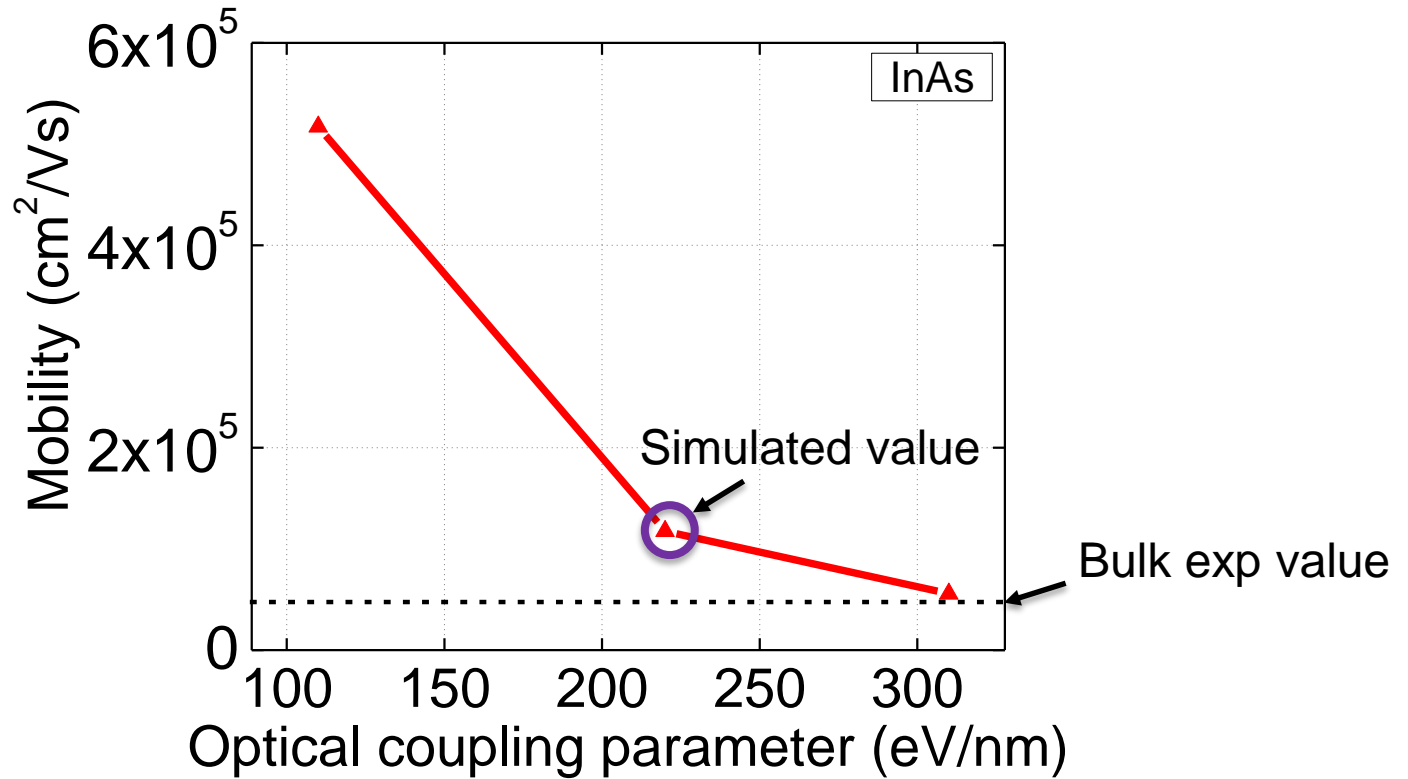
\*\*Quantum Transport in Semiconductor Nanostructures", T. Kubis PhD thesis (2009).



Region-Material	Length [nm]	Doping [cm <sup>-3</sup> ]
1 - AlSb	4.57	$3 \times 10^{19}$
2 - Al <sub>0.5</sub> Ga <sub>0.5</sub> Sb	1.2	$6 \times 10^{19}$
3 - GaSb	3.2	$5 \times 10^{19}$
4 - InAs	3.4	$1 \times 10^{15}$
5 - AlInAsSb	27.1	$1 \times 10^{15}$
6 - AlInAsSb	17.3	$5 \times 10^{19}$



Simulations and figures by Devin Verrick



Scattering strength still too weak by ~2.