UNIVERSITY of GLASGOW

Consortium Meeting
18th March 2005,

# SO phonon scattering in high-k dielectrics: the role of phonon-plasmon coupling.

John R Barker

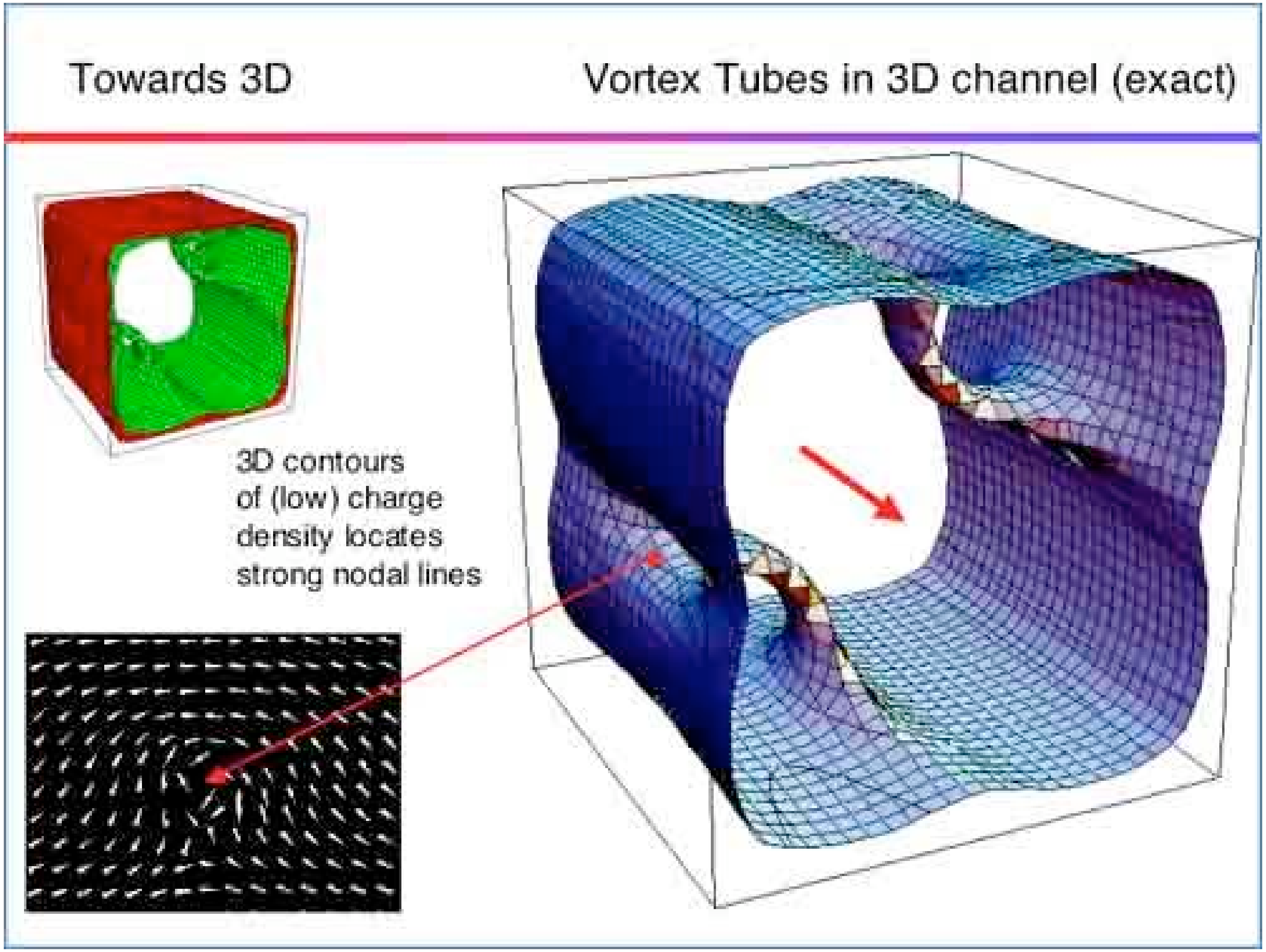
**Materials Modelling Workshop**

**University College London**

DEVICE MODELLING GROUP

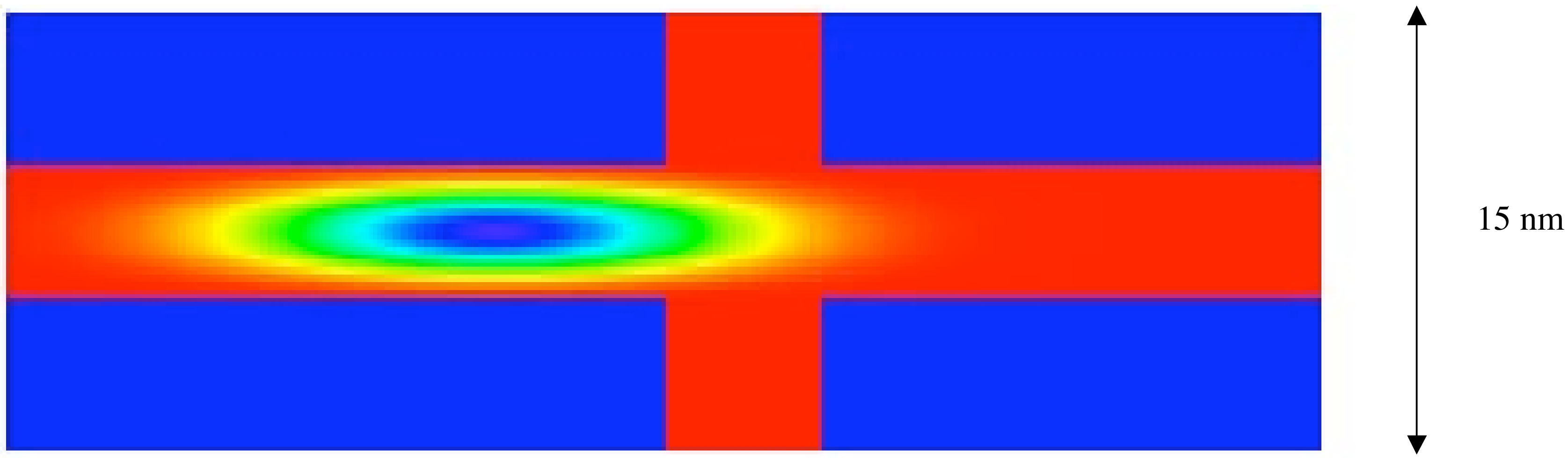
# Special request from Anantram: vortices!!

**Quantum vortices in nanowire**



# Travelling wave in transverse monomode: transmission maximum

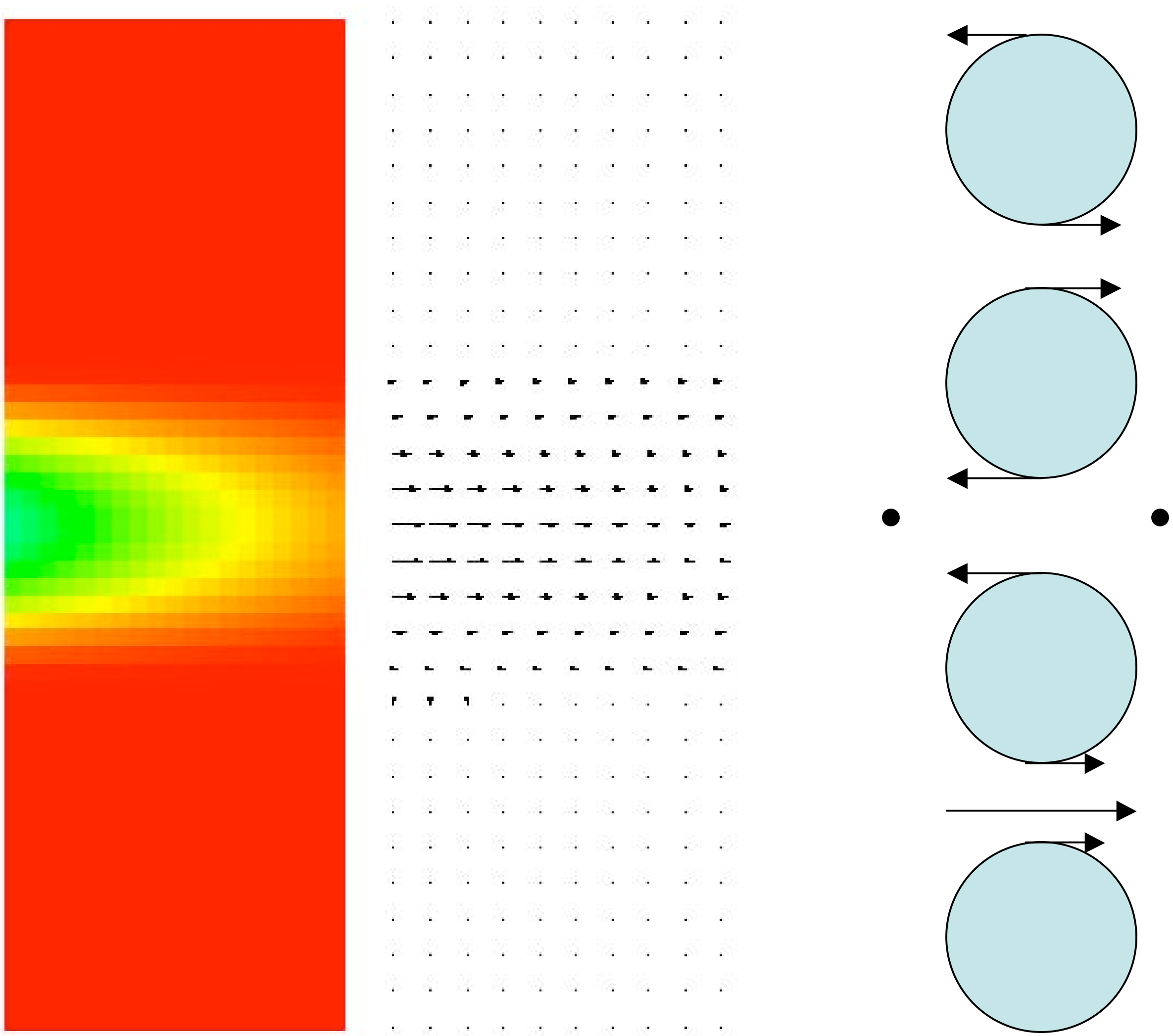
**Sharply defined energy: effect of e.g LER opening a channel: Vortex formation**




Density evolution     higher energy

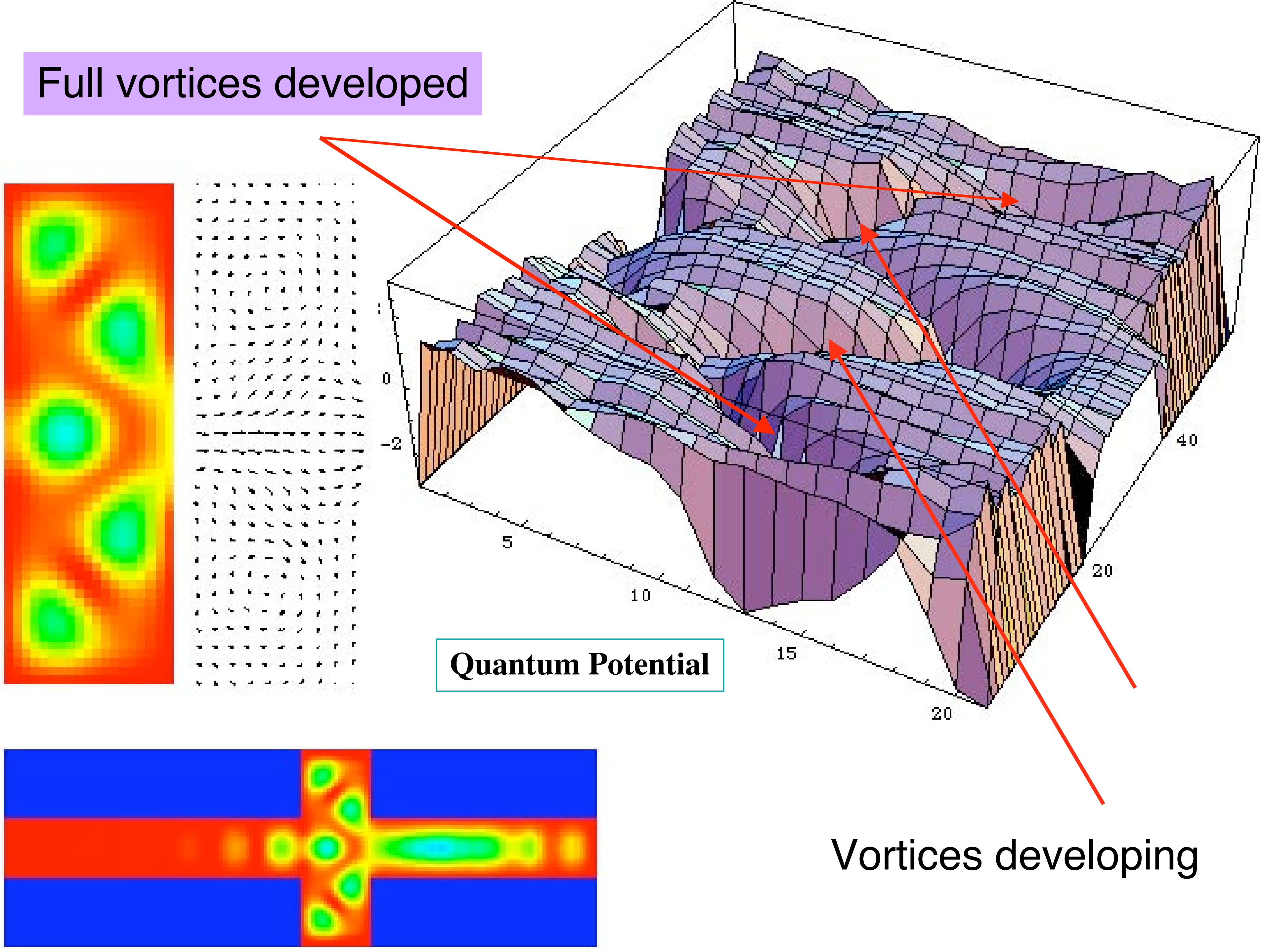
# Density & current density evolution

4 vortices formed



Transmission Maximum

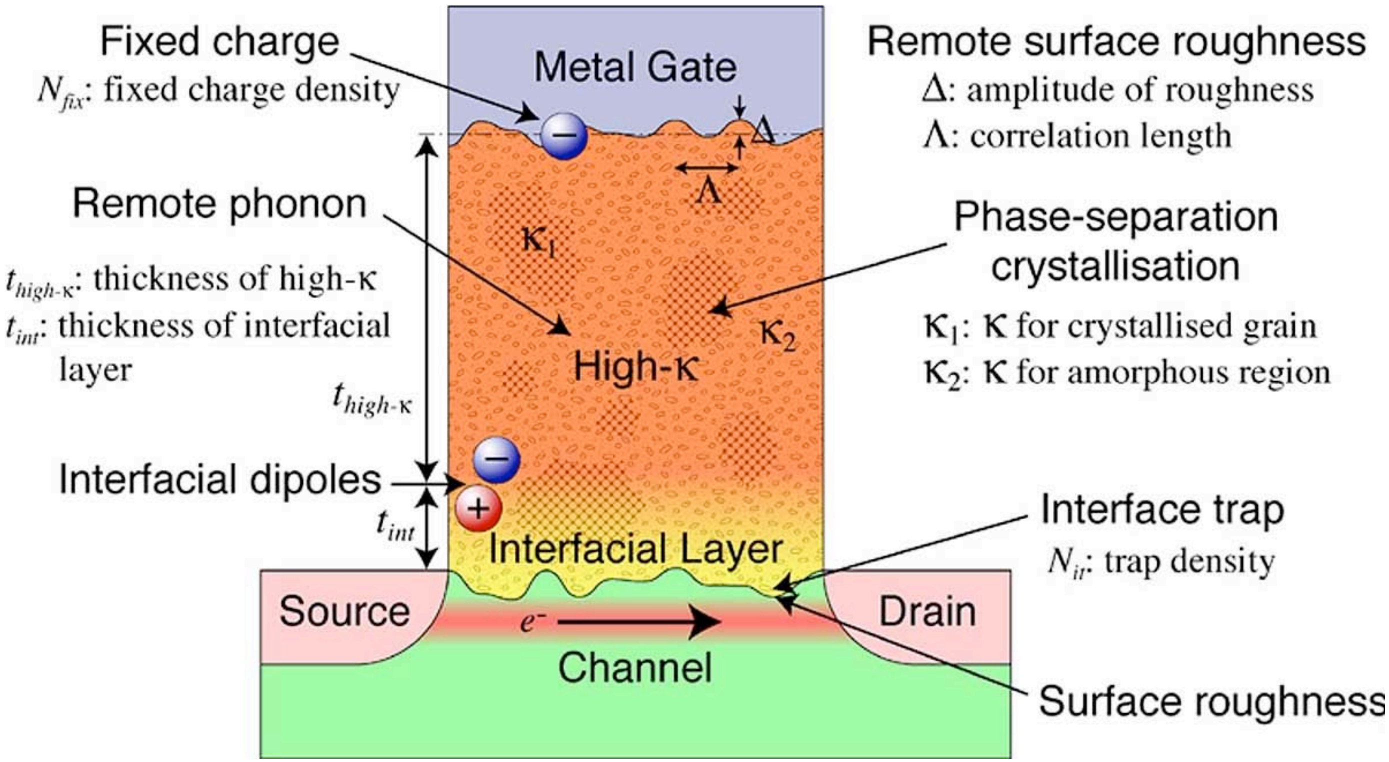
2 saddles


Full vortices developed
Quantum Potential
Vortices developing
0
-2
5
10
15
20
20
40

# Outline

- Motivation
- Background: dynamic screening
- Simple LO-phonon plasmon coupling
- Lindhard-Mermin theory
- Coulomb Drag
- Recent experimental studies
- Complex coupling: ideal high k gate stacks
- Complex coupling: non-ideal gate stacks: windowed structure
- Work in progress
- Conclusions

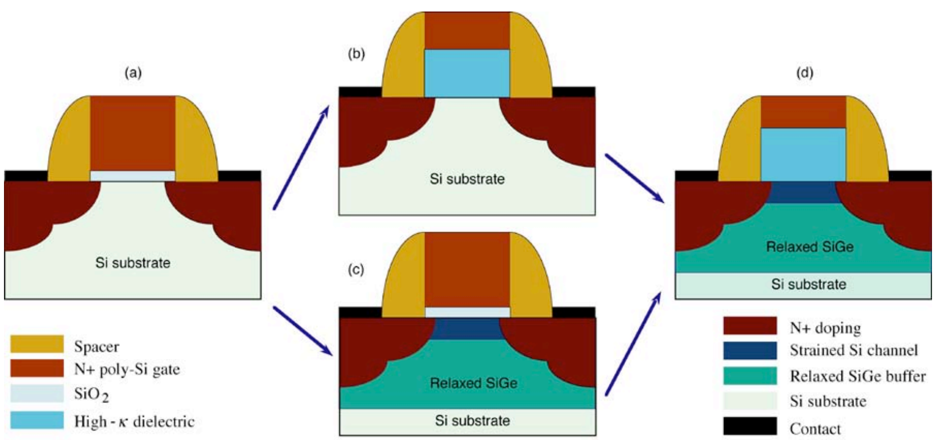
# Motivation

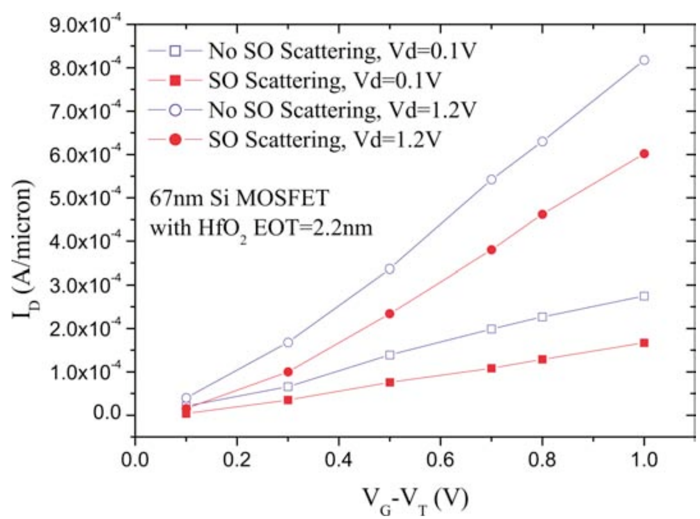


Fixed charge
$N_{fix}$: fixed charge density
Metal Gate
Remote surface roughness
Δ: amplitude of roughness
Λ: correlation length
Δ
Λ
Remote phonon
$t_{high\text{-}\kappa}$: thickness of high-κ
$t_{int}$: thickness of interfacial layer
$\kappa_1$
$\kappa_2$
Phase-separation crystallisation
$\kappa_1$: κ for crystallised grain
$\kappa_2$: κ for amorphous region
High-κ
$t_{high\text{-}\kappa}$
Interfacial dipoles
$t_{int}$
Interfacial Layer
Interface trap
$N_{it}$: trap density
Source
$e^-$
Drain
Channel
Surface roughness

It has been pointed out [1] that a severe mobility degradation ensues because of the strong coupling of carriers in the channel to surface SO phonons in the vicinity of the dielectric interface.

Recently, we have shown [2] that for ideal interfaces and homogeneous dielectrics it might be possible to offset the mobility degradation by a mobility enhancement that derives from using a strained silicon channel.



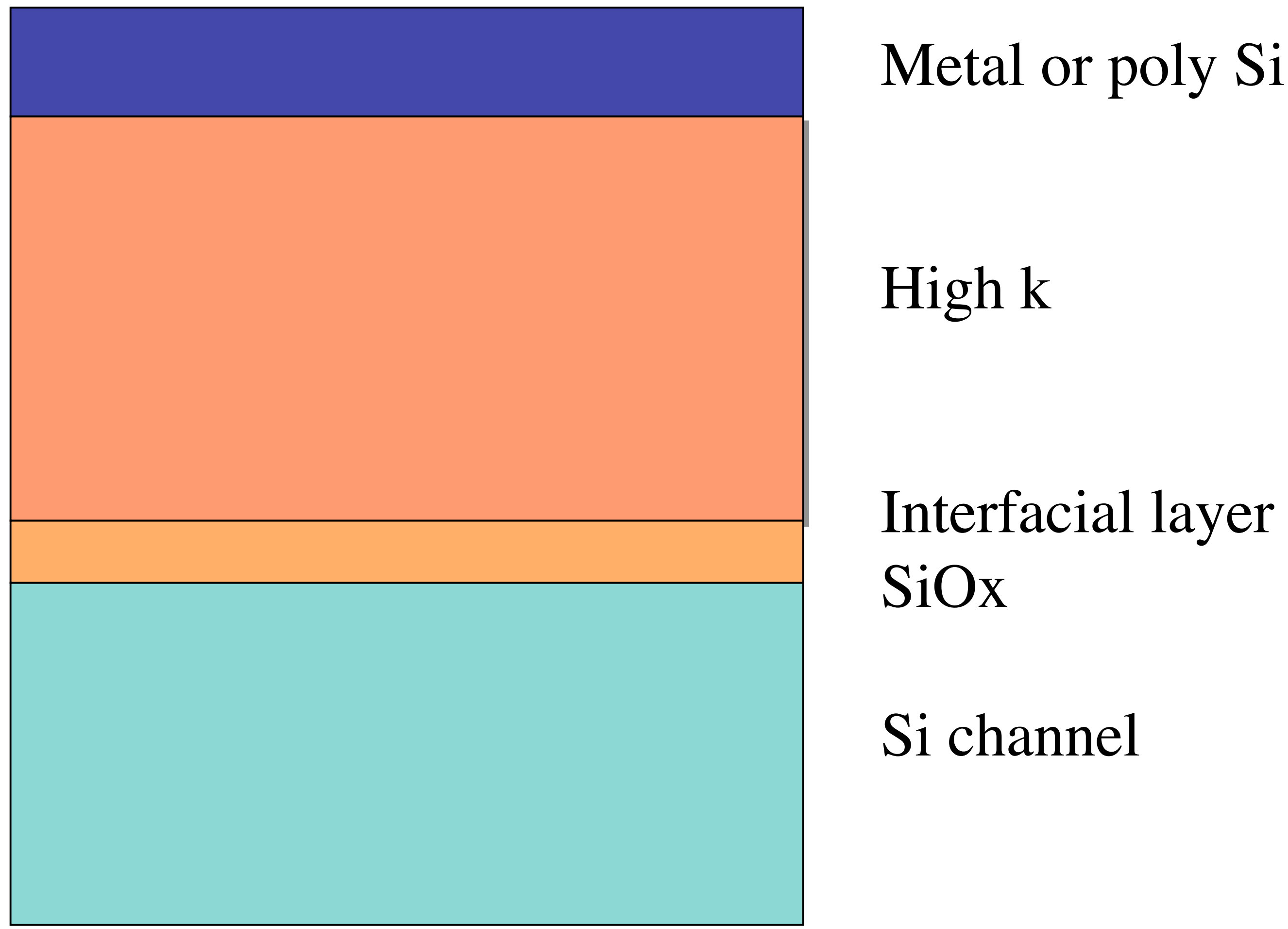



Unfortunately, the electron-phonon-plasmon scattering in such structures is a complex process that **involves the entire gate stack** through the coupling of plasmons in the gate and substrate to the phonon modes.

It is not known to what extent the electron-phonon-plasmon scattering strength is **modulated by the interface roughness** at the gate-dielectric interface and indeed, the dielectric/interfacial layer-semiconductor interface.

In addition there is evidence that many of the high κ gate stacks display significant phase separation that will distort our assessment of the spatial dependence of the scattering rates.

Finally, the understanding of the coupling problem requires an evaluation of the effects of the variation of the carrier velocity dispersion (basically electron temperature) between source and drain that acts to modulate the Landau damping of the coupled system.




Entire gate stack treated as an electrically interacting dynamical system

# 1. Naive theory: optical phonons in polar material

Lattice permittivity

$$\varepsilon_L = \varepsilon_\infty \frac{\omega^2 - \omega_L^2}{\omega^2 - \omega_T^2}$$

Lyddane-Sachs-Teller

$$\omega_L^2 = \frac{\varepsilon_S}{\varepsilon_\infty} \omega_T^2$$

Longitudinal $\quad \omega_L = 30 \quad (meV)$

Transverse $\quad \omega_T = 27.3 \quad (meV)$ GaAs

| SiO2 | Al203 | HfO2 |
|---|---|---|

Units meV

TO mode energies

| | | |
|---|---|---|
| 55.6 | 48.18 | 12.4 |
| 138.1 | 71.4 | 48.35 |

Low energies

Easily excited

Absorption as well

LO mode energies

| | | |
|---|---|---|
| 62.57 | 56.47 | 22.2 |
| 153.3 | 120.5 | 56.5 |

As emission

# 2. Basic theory: plasmons

Plasma frequency

$$\omega_P^2 = \frac{e^2 n_0}{\varepsilon_\infty m^*}$$

Dispersion

$$\omega_q^2 = \frac{q^2 < v^2 >}{3\varepsilon_\infty / \varepsilon_0} = \frac{q^2 k_B T_e}{m^* \varepsilon_\infty / \varepsilon_0}$$

Electron Permittivity

$$\varepsilon_e[q,\omega] = \varepsilon_0 - \varepsilon_\infty \frac{\omega_P^2 + \omega_q^2}{\omega(\omega - i\gamma)}$$

Pure plasmon

$$\omega^2 = \left(\frac{\varepsilon_\infty}{\varepsilon_0}\right)(\omega_P^2 + \omega_q^2)$$

# 3. Basic theory: plasmons -lifetime

Plasma frequency

$$\omega_P^2 = \frac{e^2 n_0}{\varepsilon_\infty m^*}$$

Damping
(electron scattering on
impurities
Phonons)

$$\gamma = \frac{1}{\tau} = \gamma[q]$$

$$\omega\tau > 1 \Rightarrow \text{well-defined plasma modes}$$

# 4. Basic theory: coupled modes

OK for RPA see later

Total permittivity $\varepsilon_T = \varepsilon_L + \varepsilon_e - \varepsilon_0$

For LO modes : $\varepsilon_T = 0$

*thus for* $\gamma = 0$

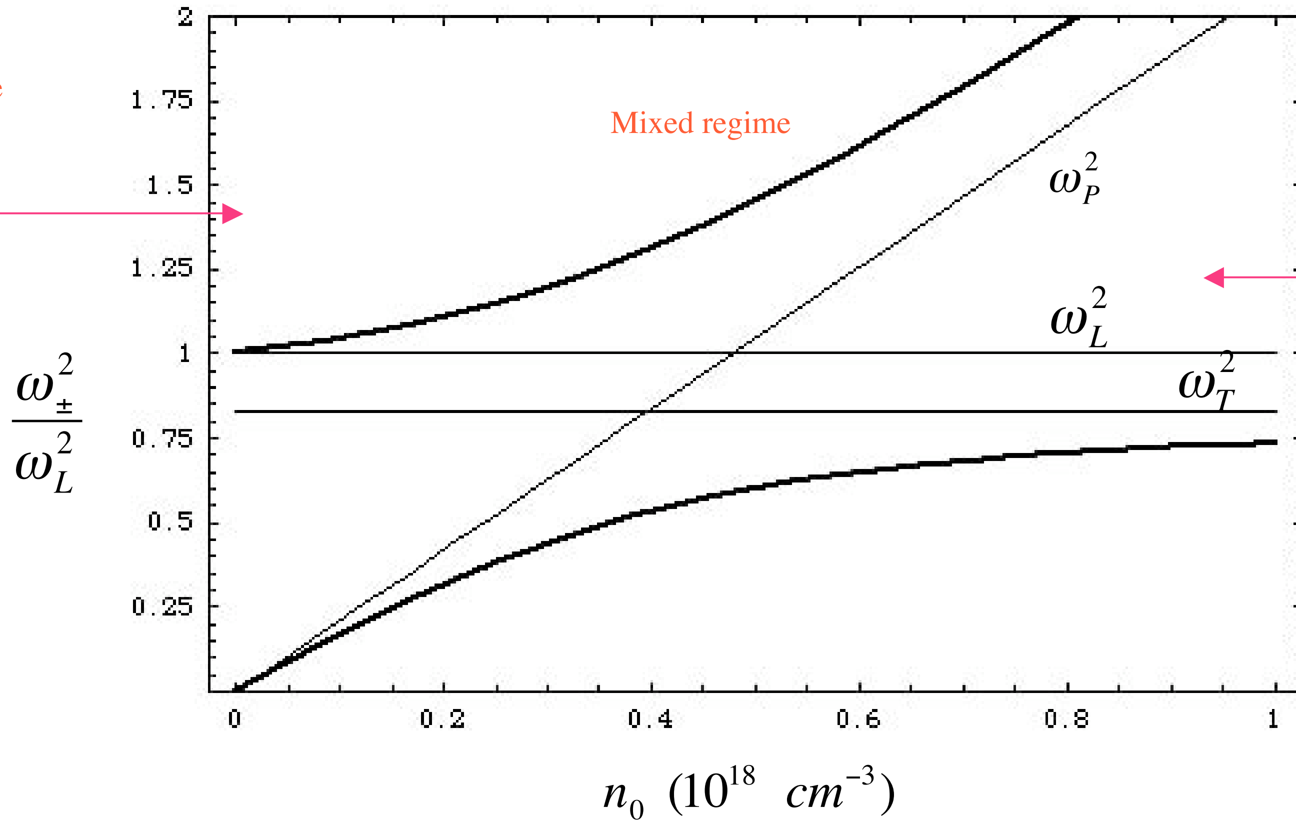
$$\omega^4 - \omega^2(\omega_L^2 + \omega_P^2 + \omega_q^2) + \omega_T^2(\omega_P^2 + \omega_q^2) = 0$$

# 5. Basic theory: coupled modes long wave limit $q = 0$

Pure
Optical mode

and

Low
frequency
Plasma
mode




Pure
plasmon

and

totally

screened optical

Mode that

Oscillates at

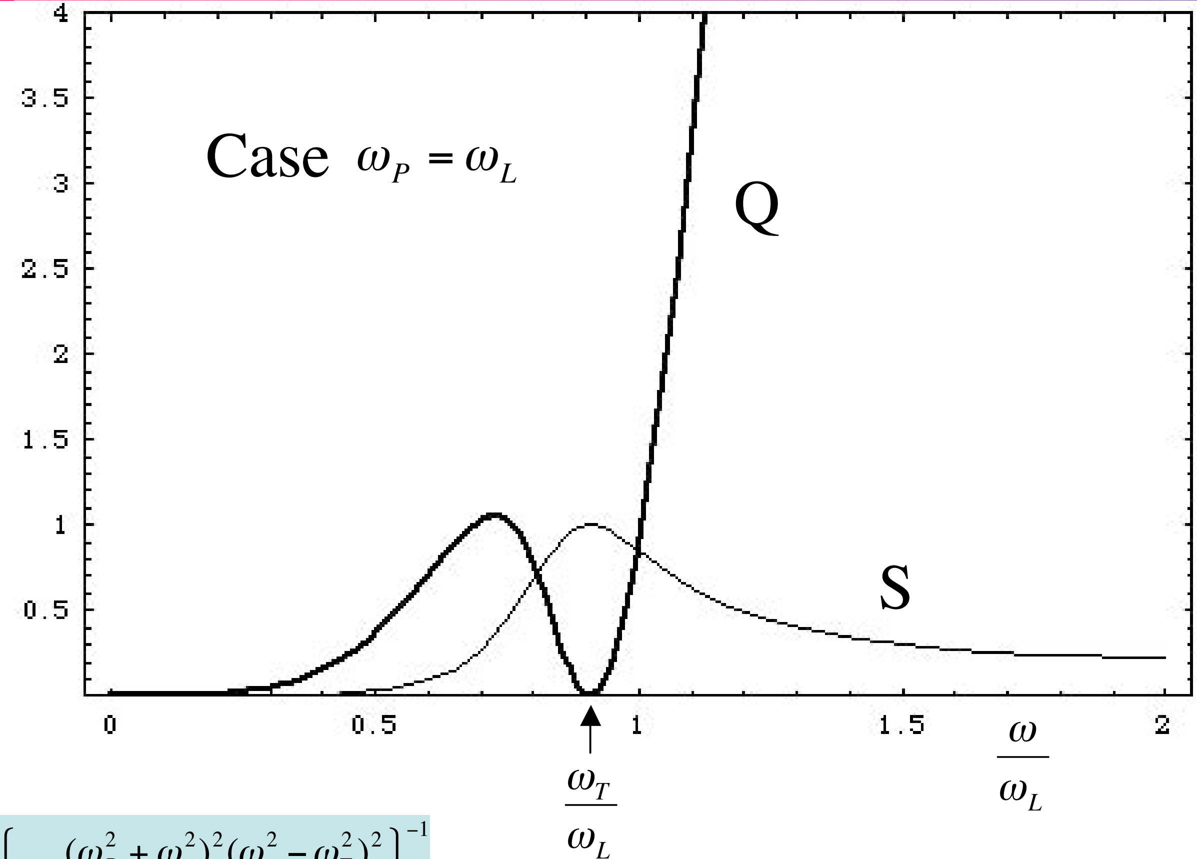
transverse mode freq

$$\omega^4 - \omega^2(\omega_L^2 + \omega_P^2) + \omega_T^2(\omega_P^2) = 0$$

$$\omega^{2+}_{-} = \frac{(\omega_L^2 + \omega_P^2) \pm \sqrt{(\omega_L^2 + \omega_P^2)^2 - 4\omega_T^2\omega_P^2}}{2}$$

GaAs
validation

# 6. Basic theory: phonon content, charge factor in long wave limit $q = 0$




Phonon content
$$S = \left\{ 1 + \frac{(\omega_P^2 + \omega_q^2)^2 (\omega^2 - \omega_T^2)^2}{\omega^4 (\omega_P^2)(\omega_L^2 - \omega_T^2)} \right\}^{-1}$$

Charge factor
$$Q = \left( \frac{(\omega^2 - \omega_T^2)}{(\omega_L^2 - \omega_T^2)} \right)^2 S$$

Coupling Strength
$$R = \frac{\omega_L}{\omega} Q$$

effective charge

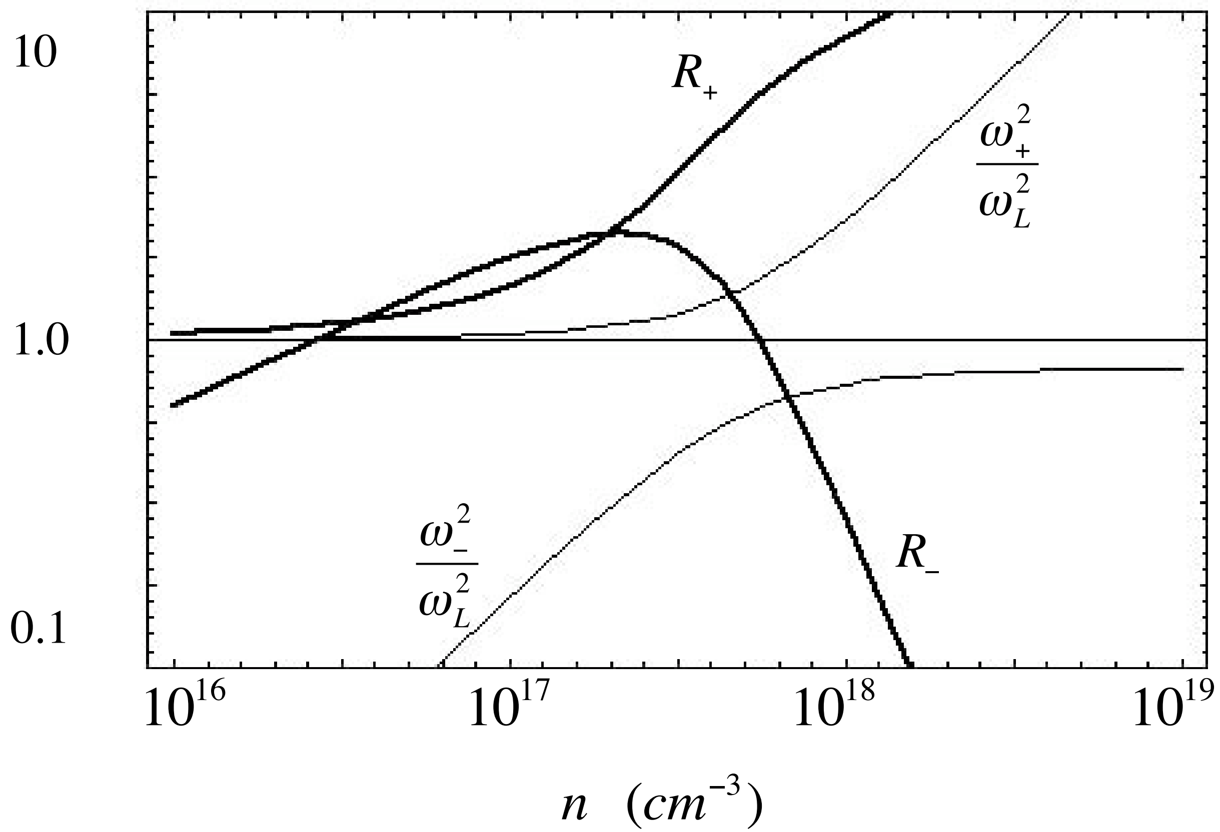
$$e^{*2} = e_L^{*2} Q$$

GaAs validation

# 7. Basic theory: effective coupling constant $q = 0$ long wavelength

Strong anti-screening

$$R = \frac{\omega_L}{\omega} Q$$




GaAs validation

Strong screening

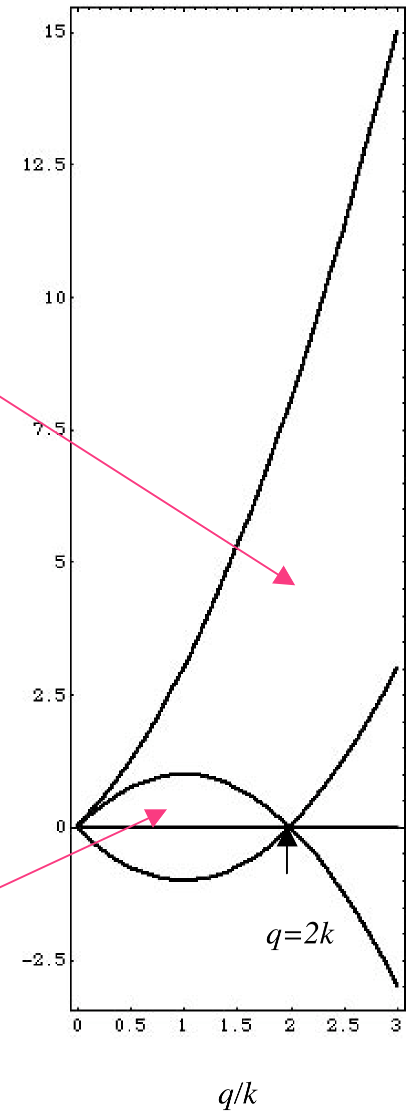
# 8. Basic theory: single particle excitation regime

*absorption*

$$\hbar\omega = \frac{\hbar^2}{2m^*}(q^2 + 2kq\cos\theta)$$

*emission*

$$\hbar\omega = \frac{\hbar^2}{2m^*}(q^2 - 2kq\cos\theta)$$




Landau damping

Units of $\frac{\hbar^2}{2m^*}$

GaAs validation

# 9. Advanced theory: Lindhard function

$$\varepsilon_e(q,\omega) = \varepsilon_0 - \frac{e^2}{q^2\Omega}\sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k+q}}) - f(\varepsilon_{\mathbf{k}})}{\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k}} - \hbar\omega - i\Gamma}$$

Describes dynamic screening, plasma oscillations,

Landau damping, collisional damping*

$$\varepsilon_e[q,\omega] = \varepsilon_0 + \left(\frac{e^2}{q^2\Omega}\right)\sum_{\mathbf{k}} f(E_k) \times$$

$$\left\{\frac{1}{E_{k-q} - E_k + \hbar\omega + i\Gamma} + \frac{1}{E_{k+q} - E_k - \hbar\omega - i\Gamma}\right\}$$

# Summary

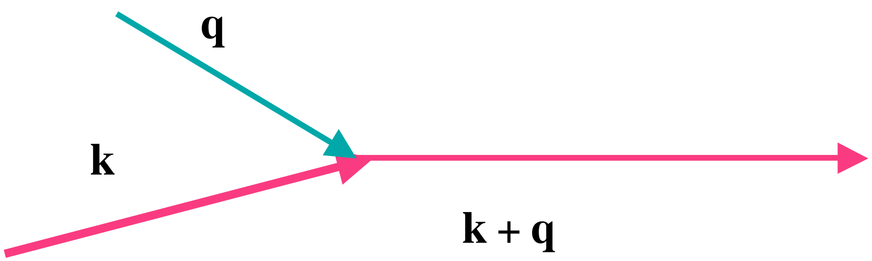
| | | | |
|---|---|---|---|
| 1. | $\omega_P << \omega_L$ | Weak screening | |
| 2. | $\omega_P \leq \omega_L$ | Anti-screening | Soft mode emerges |
| 3. | $\omega_P \geq \omega_L$ | Screening | |
| 4. | $\omega_P >> \omega_L$ | Strong screening | Entirely plasmon type |

## Screened scattering rate: Born Approximation

$$\lambda(\mathbf{k}) = \int_{-\infty}^{\infty} d(\hbar\omega)\pi^{-1}\{1 + F_{BE}(\omega)\}$$

$$\sum_{\mathbf{q}}\{1 - f(\mathbf{k}+\mathbf{q})\}\ \frac{2\pi}{\hbar}\boxed{|V(\mathbf{q})|^2\ \mathrm{Im}\{-\frac{1}{\varepsilon(q,\omega)}\}}$$

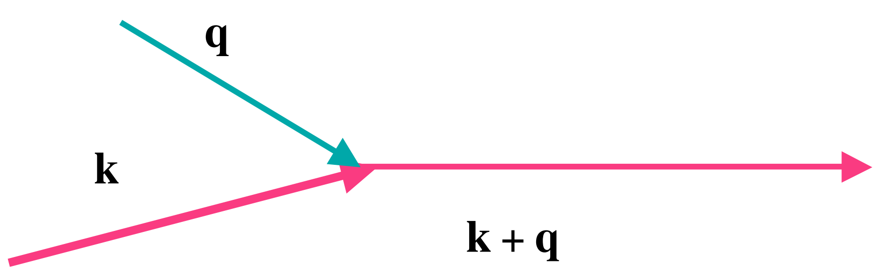
$$\delta(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \hbar\omega)$$



Screened scattering rate: Born Approximation: reduction to conventional form

$$\mathrm{Im}\{-\frac{1}{\varepsilon(q,\omega)}\} = -\mathrm{Im}\{\frac{1}{\varepsilon_\infty} - \frac{\omega_{LO}}{2}(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0})(\frac{1}{\omega_{LO} - \omega + i\eta} + \frac{1}{\omega + \omega_{LO} + i\eta})\}$$

$$= \tfrac{1}{2}\omega_{LO}\pi(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0})\{\delta(\omega - \omega_{LO}) - \delta(\omega + \omega_{LO})\}$$



# Lindhard formula in RPA

$$\varepsilon_e(q,\omega) = \varepsilon_0 - \frac{e^2}{q^2\Omega}\sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k}+\mathbf{q}}) - f(\varepsilon_{\mathbf{k}})}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \hbar\omega - i\Gamma}$$

Exact solutions at T=0,  gamma->0

q-> 0

Describes dynamic screening, plasma oscillations,

Landau damping, collisional damping*

## Summary of role of total dielectric function

Zeros of $\mathrm{Re}[\varepsilon_T(q,\omega)]$ => dispersion relation for modes

Peaks of $\mathrm{Im}[-1/\varepsilon_T(q,\omega)]$ => *microscopic energy conserving* "$\delta -$ *functions*"

Describes dynamic screening, plasma oscillations,

Landau damping, collisional damping*

# Lindhard formula in RPA: finite temperature non degenerate case

$$\varepsilon_e(q,\omega) = \varepsilon_0 - \frac{e^2 m^*}{4\pi^{3/2}\hbar q^3}\left(\frac{2m^* k_B T}{\hbar^2}\right)\{Z(A^+) - Z(A^-)\}$$

$$Z(z) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{\exp[-u^2]}{u-z}du$$

Plasma dispersion function

$$A_{\pm} = \left(\frac{2m^* k_B T}{\hbar^2}\right)^{-1}\left(\frac{m^*\omega}{\hbar q} \pm \frac{q}{2} + i\eta\right)$$

# Lindhard formula in RPA: finite temperature cases

Pade approximant for Plasma dispersion function

Essential to handle Monte Carlo numerics

$$Z(z) = \frac{i\sqrt{\pi} + (\pi - 2)z}{1 - i\sqrt{\pi}z - (\pi - 2)z^2}$$

D. Lowe and J.R. Barker (1985)

Degenerate case now derived

J.R.Barker 2005

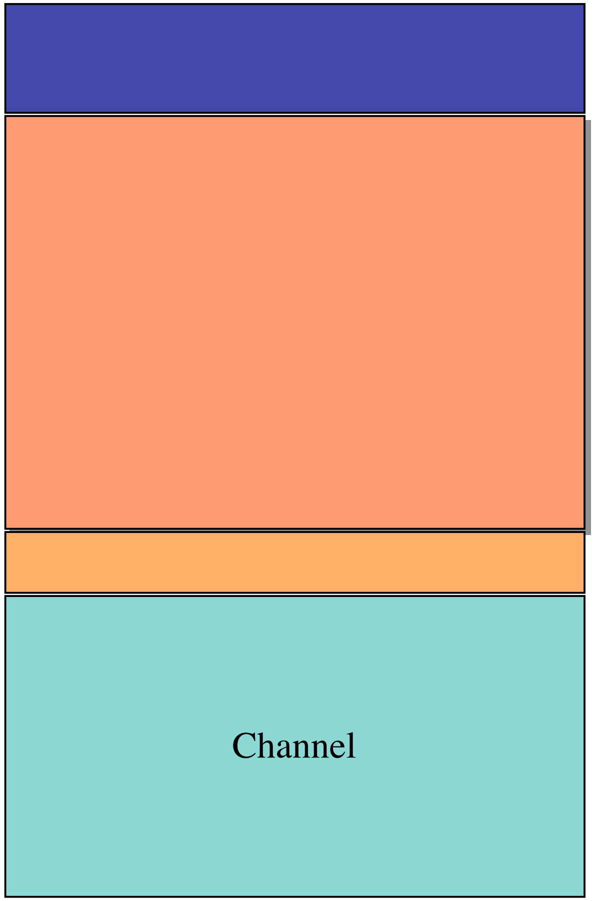
## Long Range remote scattering in FETs

**Remote scattering**:

Impurities in gate interact with electrons in channel

Electrons in gate interact with electrons in Channel. **Coulomb drag**

Enhanced by plasmon interactions in the gate.



Momentum transfer between non-equilibrium carriers in channel and equilibrium carriers in gate.

Fischetti J.App.Phys. 89 1232 (2001)

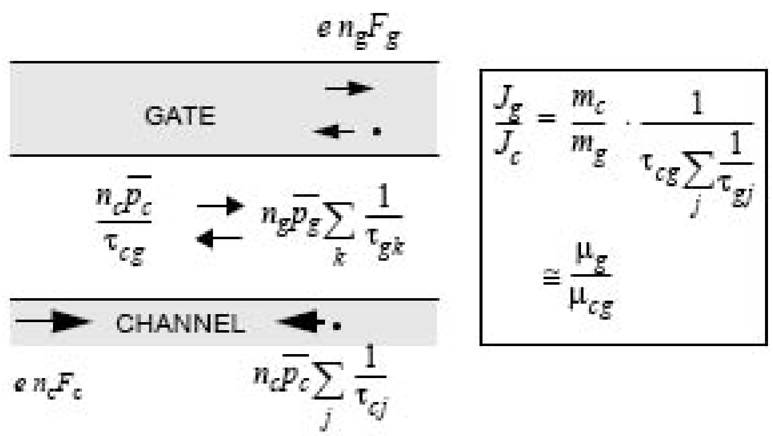



Fig. 1. Drag momentum transfer equations. Symbol key, subscripts $x$ = $c$ or $g$ refer to channel or gate respectively: $e$ = electronic charge, $n_x$ = sheet electron concentration, $m_x$ = electron effective mass, $\tau_{xj}$ = relaxation time due to $j^{th}$ scattering process, and $\bar{p}_x$ = mean electron momentum. $F_c$ = driving electric field in channel, $F_g$ = induced field in gate, $\mu_g$ = mobility in gate, and $\mu_{cg}$ = the gate-induced mobility in the channel.

From
Solomon and Yang
(2005)

## ❑Recent experimental studies

**Relevance of Remote Scattering in Gate to Channel Mobility of thin-oxide CMOS devices.**

Paul M. Solomon and Min Yang

IBM Semiconductor Research and Development Center: Research Division,

T.J. Watson research Center, Yorktown Heights, NY 10598,

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IEDM 2004

**Abstract**

Coulomb drag between electrons in the channel, and electrons in the gate was measured for the first time on silicon MOSFETs having different gate oxide thicknesses and polysilicon doping levels. These measurements were augmented by mobility measurements in both the channel and the gate. The drag results showed current transfer ratios between channel and gate of ~$2\times10^{-4}$, and not to be a strong function of oxide thickness in the 1.9-2.8 nm range. The derived transfer mobility between channel and gate is ~$1.5\times10^{4}$ cm$^2$/V-s, too large to significantly affect channel current. We show also that neither drag nor remote impurity scattering can account for mobility degradation observed on our thinner oxide samples.

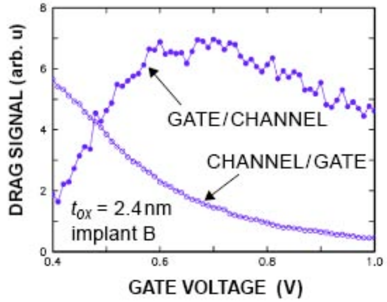



Fig. 5. Drag voltage measured on gate (●) and channel (o) with signal applied to channel and gate. Full scale = 0.1 and 5μV respectively

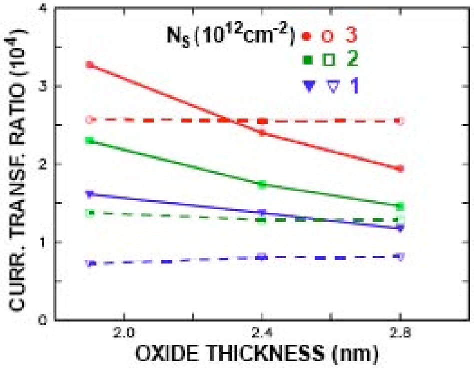



Fig. 10. Channel/gate current transfer ratio vs. oxide thickness for implants D (solid) and C (dashed) and for different channel electron concentrations as indicated.

**Implications**

The strong plasmon enhanced drag predicted by Fischetti. [1] is not seen. Our values for current transfer ratio and gate mobility yield a transfer mobility, $\mu_{cg}=A_I/\mu_g$, of ~15,000cm$^2$/V-s for our 1.9nm oxide, which would not cause significant mobility degradation in the FET channel. This is most likely a consequence of the very strong scattering in the polysilicon, which prevents plasmons from forming. This, coupled with the weak thickness dependence (see Fig. 10), is good news implying that gate-induced drag will not limit mobility for even thinner oxides. Drag may be still important, as pointed out by Fischetti, between the channel and S/D regions.

# Damping of plasma oscillations

The IBM data may be interpreted as due to strong scattering in the poly-silicon gate leading to a **collisional broadening of the Lindhard function**.
If $\tau_C$ is the collision rate the simplest extension to Lindhard formula that conserves particle number is:

$$\varepsilon_e[q,\omega] \rightarrow \varepsilon_0 + \frac{(1 + i/\omega\tau_c)(\varepsilon_e[q,\omega] - \varepsilon_0)}{1 + (i/\omega\tau_c)\dfrac{(\varepsilon_e[q,\omega] - \varepsilon_0)}{(\varepsilon_e[q,0] - \varepsilon_0)}}$$

**Strong collisional broadening**

c.f Mermin (1970)

$$\omega\tau_c << 1 \qquad \varepsilon_e[q,\omega] \rightarrow \varepsilon_e[q,0]$$

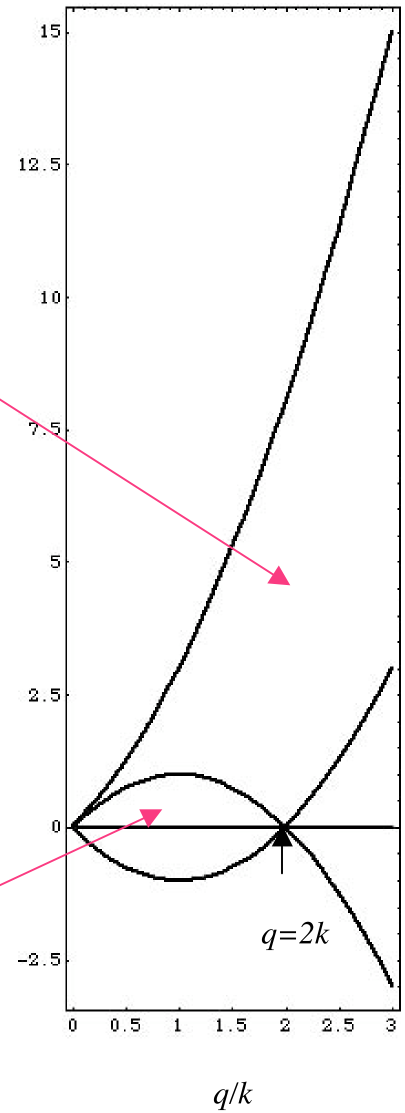
# single particle excitation regime

*absorption*

$$\hbar\omega = \frac{\hbar^2}{2m^*}(q^2 + 2kq\cos\theta)$$

*emission*

$$\hbar\omega = \frac{\hbar^2}{2m^*}(q^2 - 2kq\cos\theta)$$




**Landau damping**

**Undamped region**

Modes well-defined

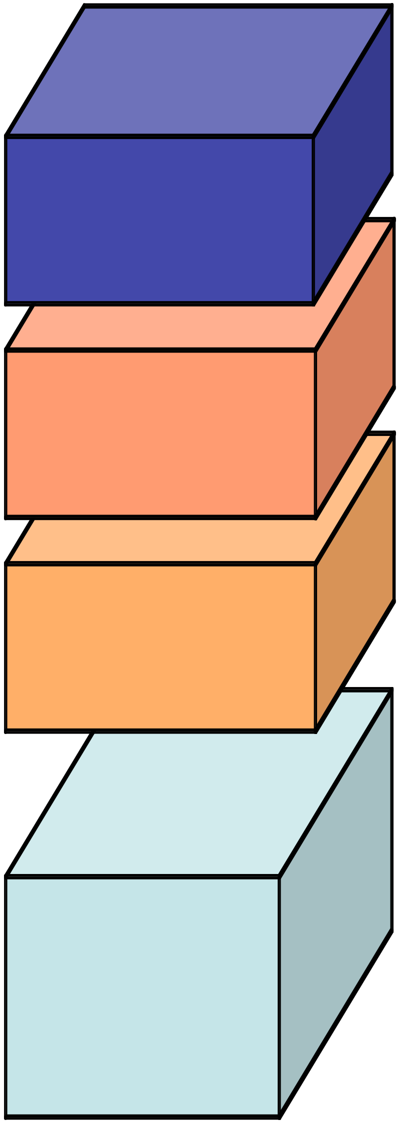
**Damped region**

Modes not well-defined

Get different dispersion relation

"Lorentzian style"
Spectral density of states
Rather than "delta functions"

## Complex coupling: ideal high k gate stacks



Plasmons in gate and substrate couple to interface phonons

and dynamic screening of remote impurity/electron/phonon scattering

Basic approach established by

Kim, Das and Senturia Phys.Rev B 18 6890 (1978)
Fischetti J.App.Phys. 89 1205 (2001)
Fischetti and Laux, J.App. Phys. 89 1232 (2001)
Fischetti, Neumayer, Cartier, J.App.Phys. 90 4587 (2001)

# Complex coupling: ideal high k gate stacks

Electrostatic potential

$$\varphi(\mathbf{R}, z, t) = \sum_{\mathbf{Q}} \varphi_{Q\omega}(z) \exp[i(\mathbf{Q}.\mathbf{r} + \omega t)]$$

$$\frac{\partial^2 \varphi}{\partial z^2} - Q^2 \varphi = 0$$

Poisson eqn
Reduces to
Laplace eqn
Reduces to
Helmholtz eqn

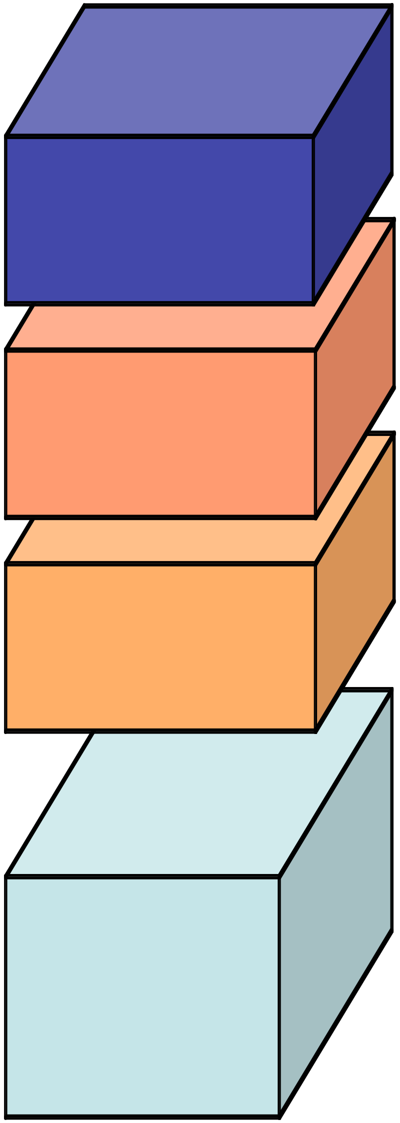
$$a_0 \exp[Q(z - t_0)]$$

$$a_1 \exp[Q(z - t_0)] + b_1 \exp[-Q(z - t_0)]$$

$$a_2 \exp[Q(z - t_0)] + b_2 \exp[-Q(z - t_0)]$$

.......

$$b_n \exp[-Q(z - t_0)]$$



2 BoundaryConditions
at each interface introduces
dielectric functions

Set of sim. Eqns

Vanishing determinant
For solution
=> Dispersion relation

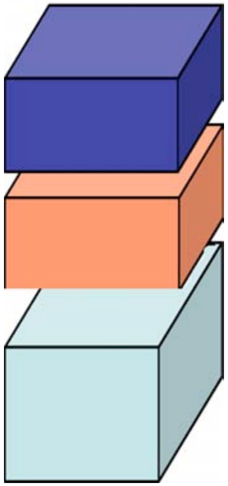
Simple matching: transfer matrix

# Dispersion relation

Example: Gate-dielectric-silicon

$$\varepsilon^2{}_{hk}(\omega) + \varepsilon_{hk}(\omega)\{\varepsilon_{gate}(\omega) + \varepsilon_{si}(Q,\omega)\}Coth[Q(t_1 - t_0)]$$
$$+\varepsilon_{gate}(\omega)\varepsilon_{si}(Q,\omega) = 0$$

$$\omega = \omega(Q)^{(j)} \qquad j = 1\ldots6$$



Six modes: 2 are weak scattering associated with TO modes

The rest are coupled plasmon-phonon modes

In the Landau damping region the plasma oscillations are damped

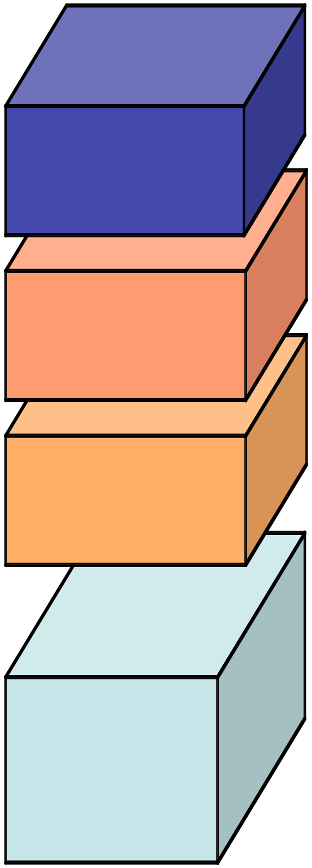
Alters scattering strength and energies

## ❑Dispersion relation

Example2: Gate-dielectric-interfacial layer-silicon

$$(\varepsilon_{gate}+\varepsilon_{hk})(\varepsilon_{si}+\varepsilon_{oxide})(\varepsilon_{hk}+\varepsilon_{oxide})$$
$$+(\varepsilon_{gate}-\varepsilon_{hk})(\varepsilon_{si}+\varepsilon_{oxide})(\varepsilon_{oxide}-\varepsilon_{hk})\exp[-Q(t_1-t_0)]$$
$$-(\varepsilon_{gate}+\varepsilon_{hk})(\varepsilon_{si}-\varepsilon_{oxide})(\varepsilon_{oxide}-\varepsilon_{hk})\exp[-Q(t_2-t_0)]=0$$

$$\omega=\omega(Q)^{(j)} \qquad j=1\ldots16$$



Sixteen modes: 4 are weak scattering associated with TO modes, 2 in each insulator.
The 12 remaining are coupled plasmon-surface phonon modes

In the Landau damping region the plasma oscillations are damped

To treat Landau damping and collisional damping we use Lindhard function

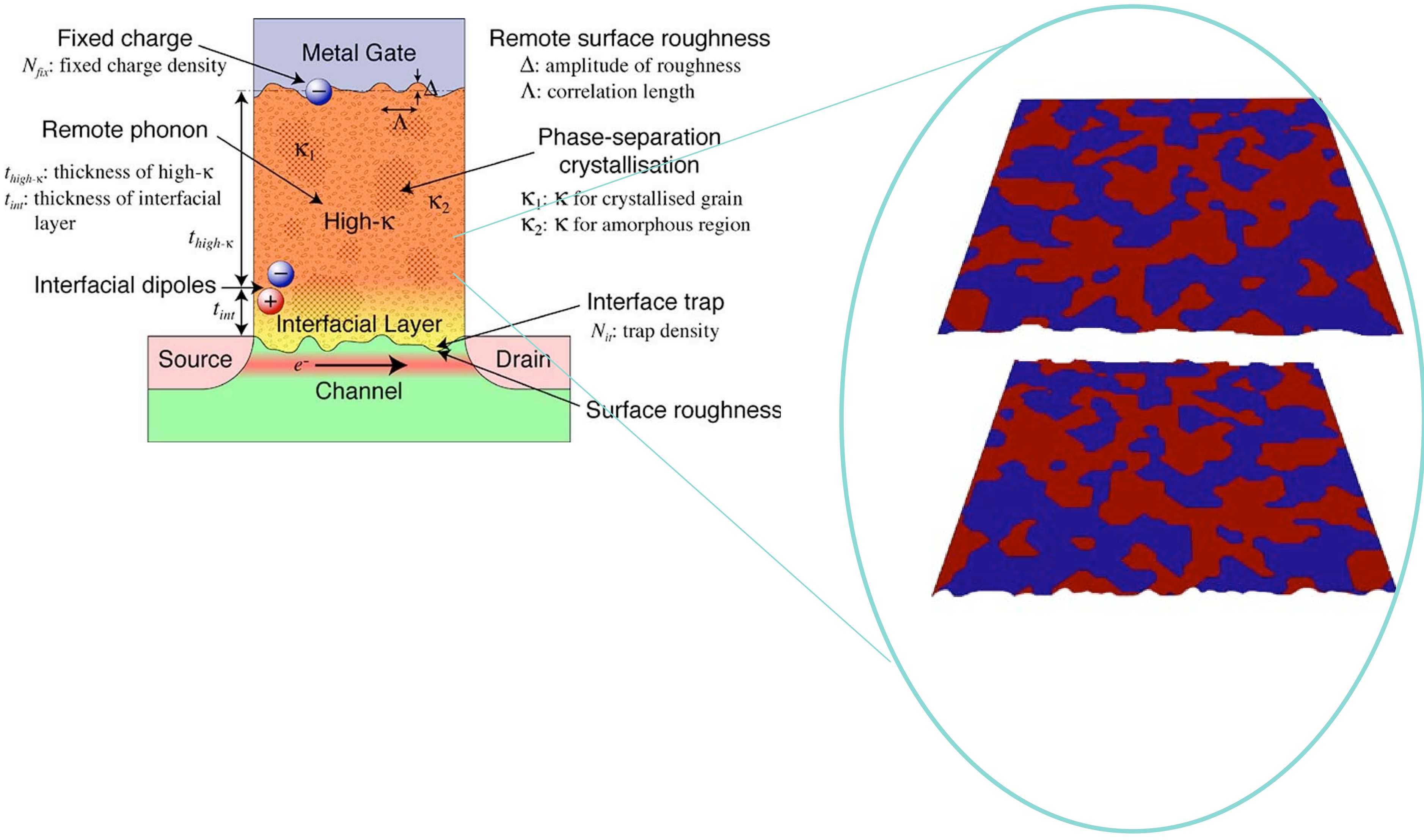
**Interfacial layer reduces strength of SO scattering by**

$$\exp[-Qt_{\text{interfacial}}]\sim\exp[-2k_F t_{\text{interfacial}}]$$

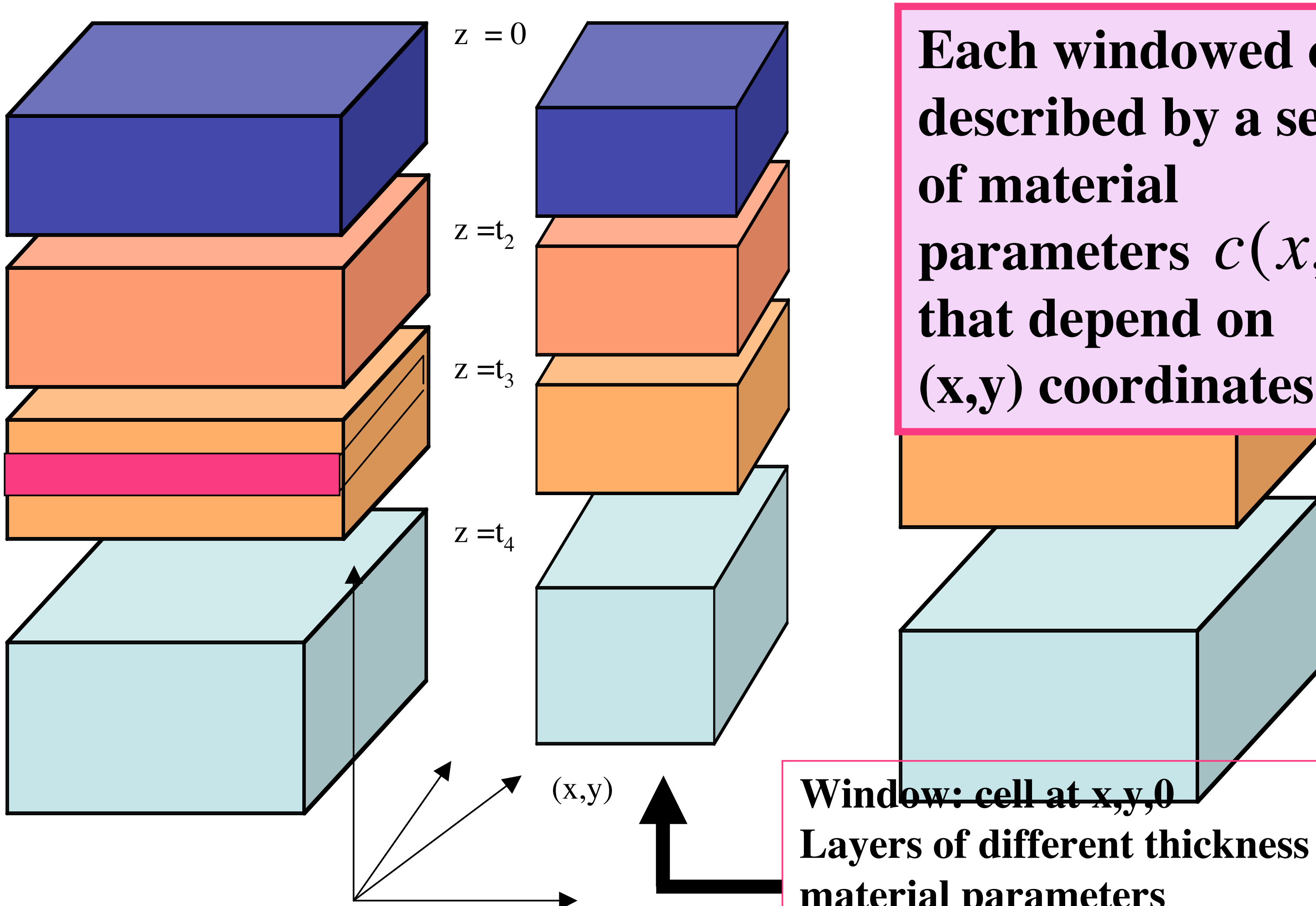
Low n needs thick layer

High n thin layer OK

## Complex coupling: non-ideal gate stacks:



## Complex coupling: non-ideal gate stacks: windowed structure




**Each windowed cell described by a set of material parameters $c(x, y, z')$ that depend on (x,y) coordinates**

**Window: cell at x,y,0**
**Layers of different thickness and material parameters**
**2D or 3D model, extendable to S and D**

# Examples of cell parameters *c(x,y)*

Dynamics: effective mass m* (tensor) $m^*(x,y,z) : z \in (t_n, t_{n+1})$

Electron temperature $T_e(x,y)$

Material type

Ionic Dielectric properties

Layer thicknesses

Bare Phonon frequencies

Coupling constants

Windowing involves a filter function
c.f DWFT
D Wilson-Zak transform

Allows correction and/or smoothing
Artefacts from finite cells

Neglects fringing effects at S and D

Overcome by frozen field?

**At silicon level** :

Dynamically Screened Scattering Rate $\lambda[\mathbf{k}, x, y, z \mid c(x, y, z')]$

Electron temperature $T_e(x,y)$

Plasma frequency depends on n.

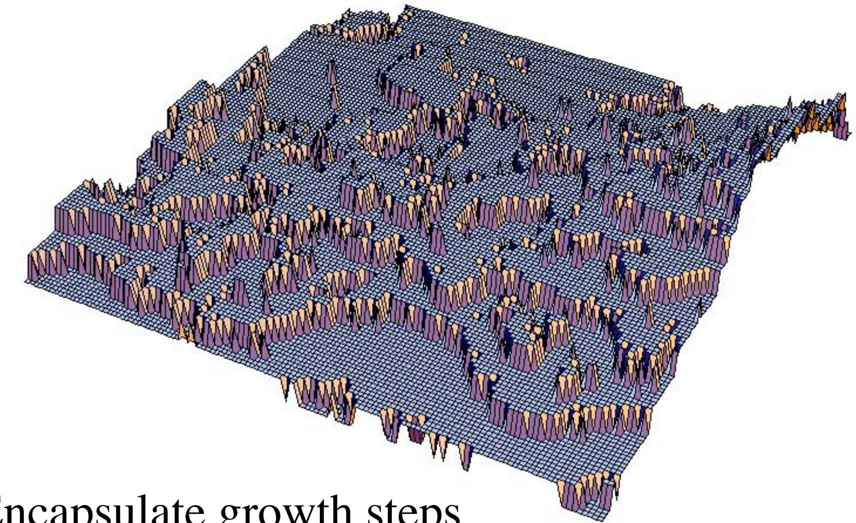
Dominant effects:

Modulation of dynamically screened SO interaction and Coulomb drag by interface roughness at each interface.

$$\frac{1}{\tau} \sim \sum_{q} \exp[-q < t >] . \frac{(1 - q\Delta t(\mathbf{r})/2)}{(1 + q\Delta t(\mathbf{r})/2)} \ldots$$

Modulation of dynamically screened SO interaction and Coulomb drag by local electron density and electron temperature in channel.

# Fractal models of interfaces and phase separation



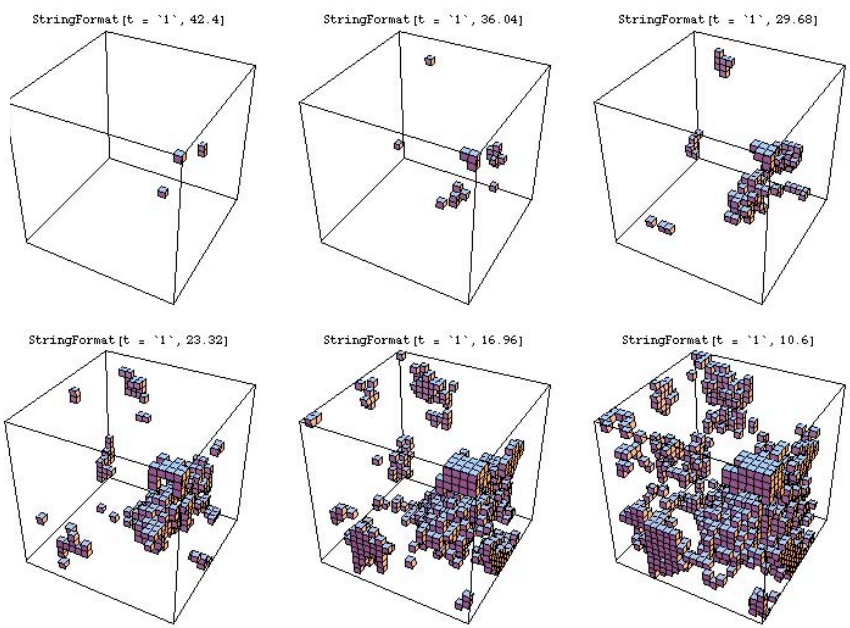
Seed with generic shapes

Could be used as a growth model

Encapsulate growth steps
“Molecular shapes” of
typical disorder patterns

Explore different topgraphies

With same exptal rms height
and correlation length



# Work in progress

- Validation of idealised gate stack theory
  -coupled phonons-plasmons, scattering rates

- Lindhard formula: fast algorithm for degenerate case

- Damped Lindhard model: Landau and Collisional

- Port to Monte Carlo 2D/3D

- Port of non-ideal gate stack theory

- Surface roughness scattering modulated by
  plasmon-enhanced SO phonon scattering

- 3D Fractal model for mixed phase dielectric-Sematech data?
- 3D Fractal model for interfaces- build in features from UCL?
  -generate "typical" structures.

- Construction of "typical" local mobility map-> Drift Diffusion?

## Conclusions

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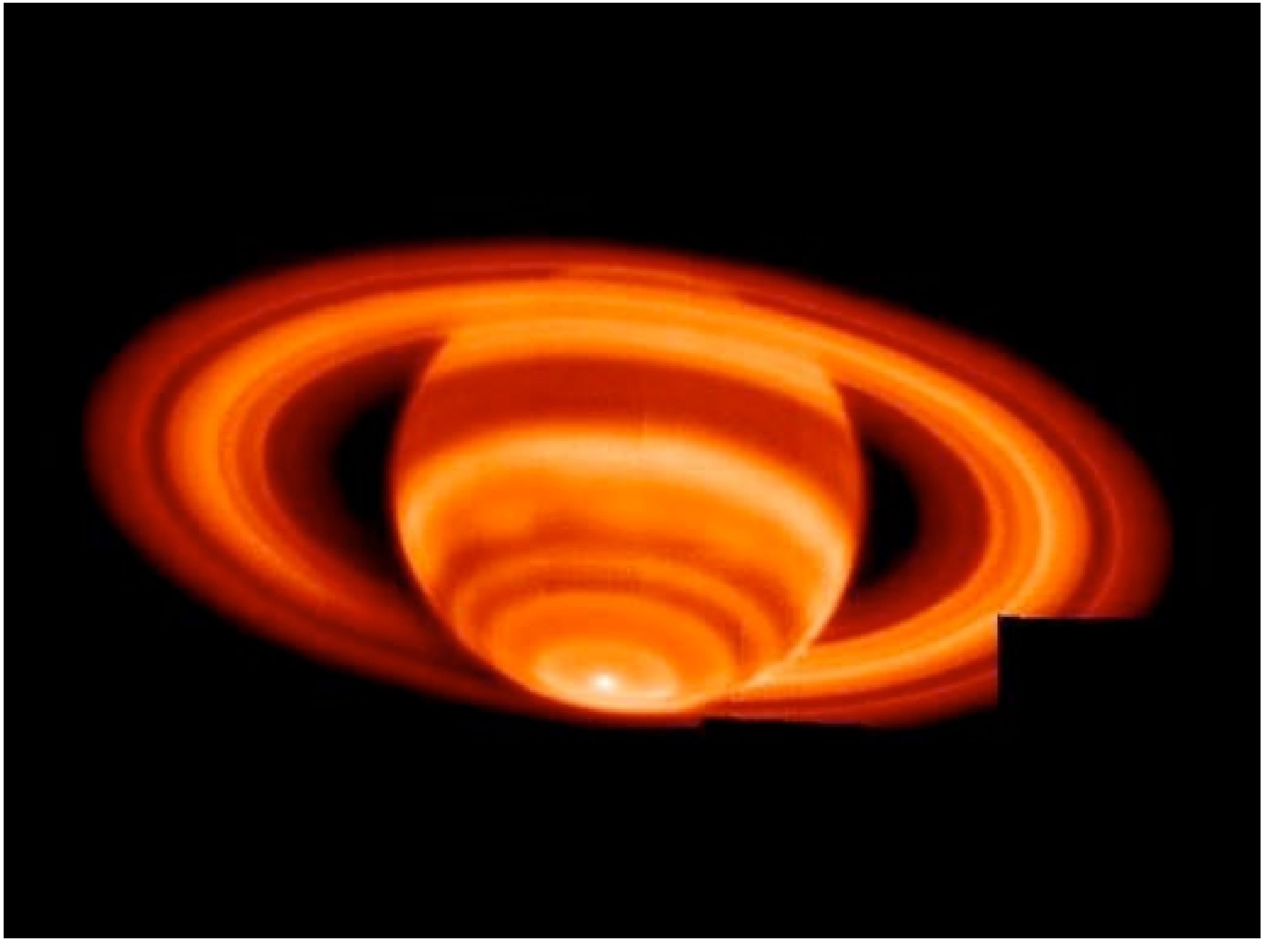
- Extended Fischetti style theory to realistic structures
- Include space dependent electron temperature for degenerate electrons
- Introduce damped Lindhard-Mermin function-new algorithms
- Landau damping and collisional damping
- Interface roughness at each interface modulates SO phonon scattering
- Spatial dependence of key parameters such as coupled phonon/plasmon frequencies
- Using windowed cell method.
- Multi-layer dielectric theory
- Fractal models
- **Mobility map to assess devices by DD**.
- Future: use secondary self scattering for fast MC computation.



Biggest vortex in solar system!