Second GreEnergy workshop - Wideband optical antennae for use in energy harvesting applications

Monte Carlo simulations of graphene ballistic diodes

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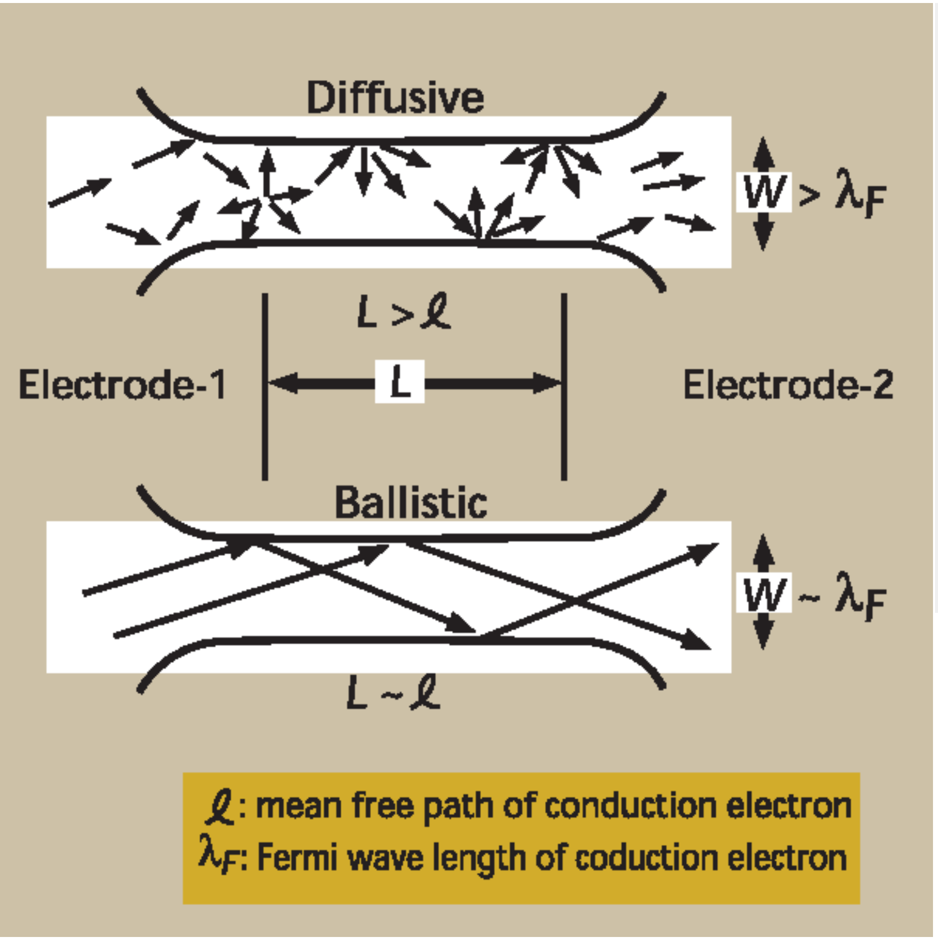
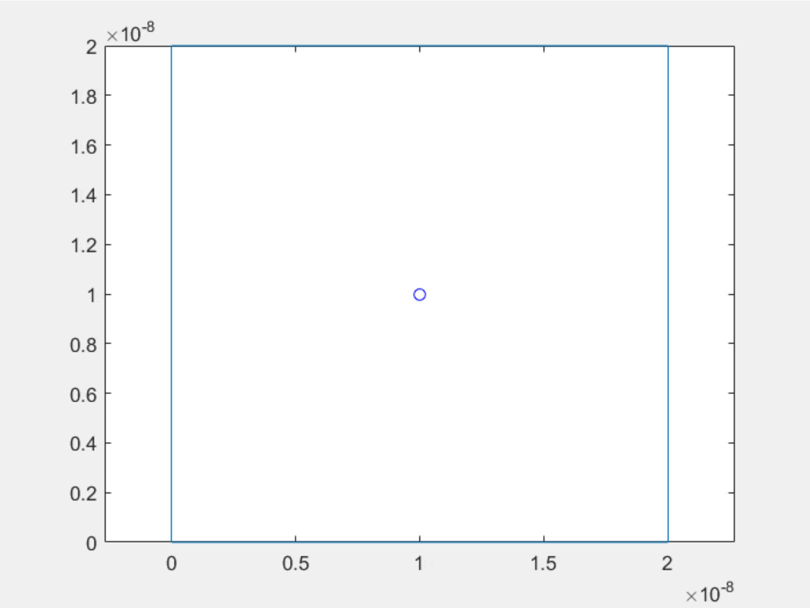
Outline

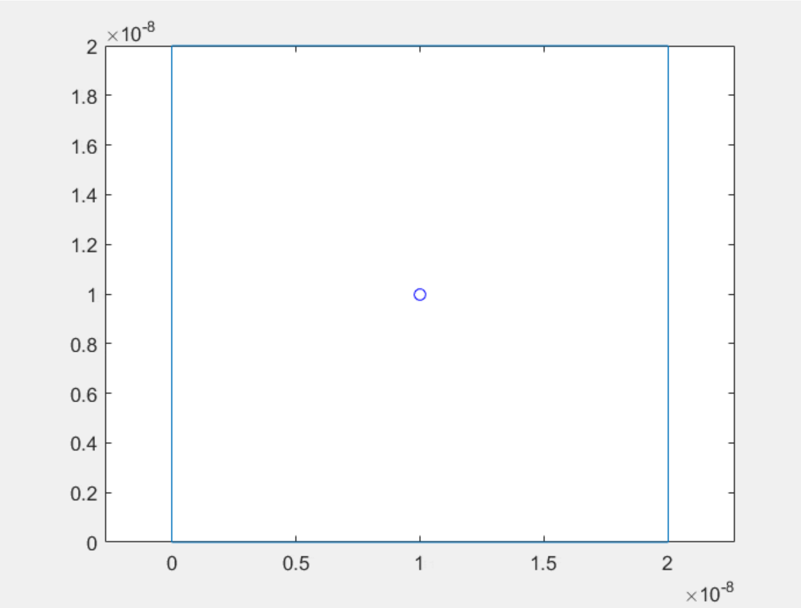
- **Introduction**
- Model description
- Results
- Conclusion

Introduction: Ballistic transport





Ballistic transport

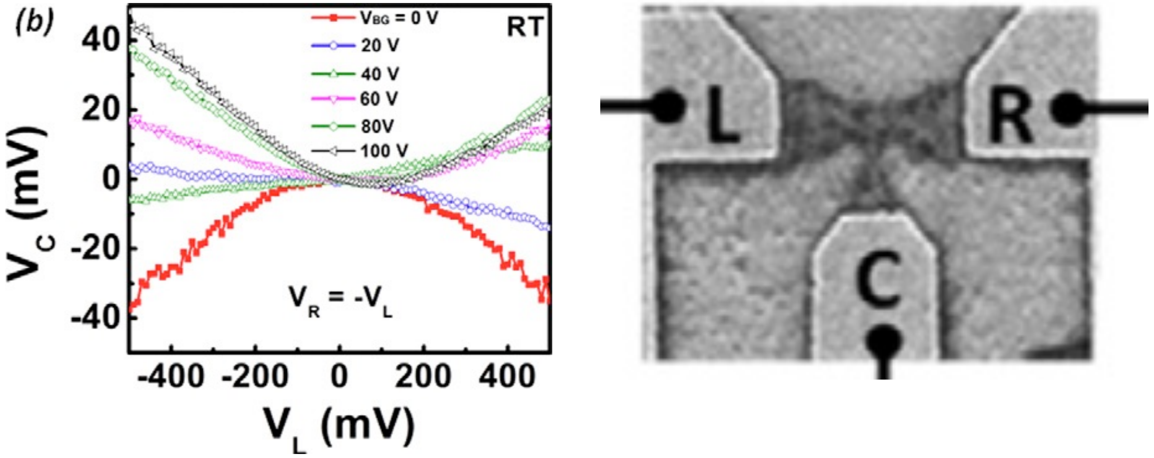


Diffusive transport

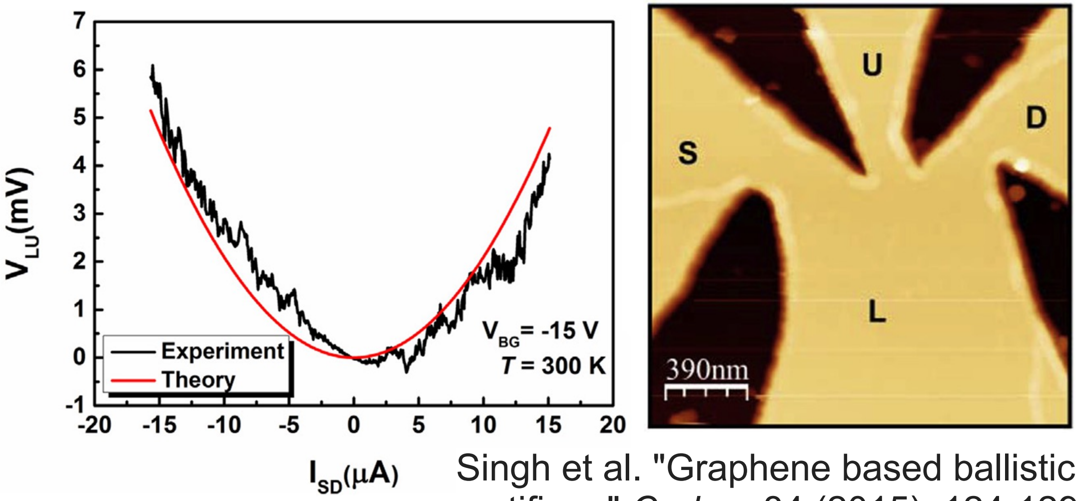
- In ballistic regime carrier’s trajectory can be modified by device geometry

Takayanagi, Kunio, Y. Kondo, and H. Ohnishi. "Suspended gold nanowires: ballistic transport of electrons." JSAP int 3.8 (2001)..

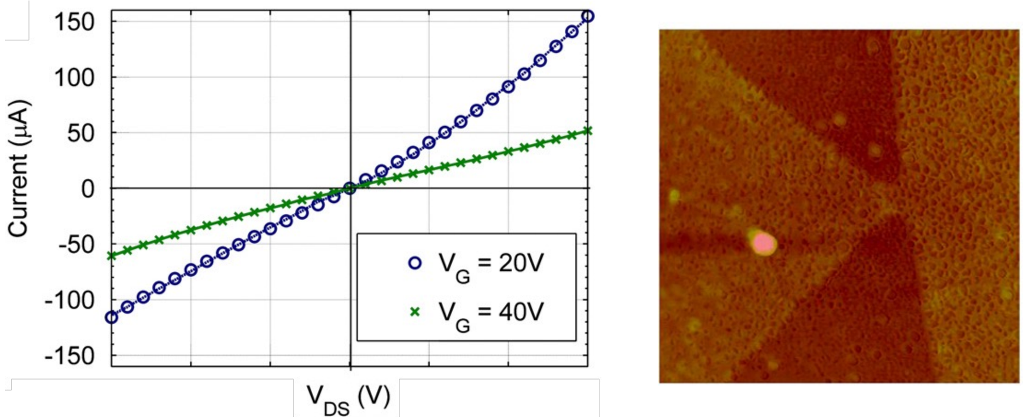
Introduction: Ballistic diodes



Kim et al. "Nonlinear behavior of three-terminal graphene junctions at room temperature." *Nanotechnology* 23.11 (2012): 115201.



Singh et al. "Graphene based ballistic rectifiers." *Carbon* 84 (2015): 124-129.



Moddel et al. "Ultrahigh speed graphene diode with reversible polarity." *Solid State Communications* 152.19 (2012): 1842-1845.

- Graphene structures with geometrical asymmetry
- Rectification a non-linear effect arising from geometrical features and it is favoured by ballistic transport conditions
- Experimental results demonstrates the non-linear behavior

Introduction: Graphene ballistic diodes

- **No built-in potential/space charge region**
  - No threshold voltage → small signal rectification
  - No parasitic capacitance → high frequencies rectification
- **Experimental evidence**
  - Capacitance estimation ≈aF & rectification up to 28 THz for 2 terminal device [1]
  - THz imaging for 4 terminal device [2]

- **Energy harvesting applications**

- **Why graphene?**
  - Need ballistic transport
  - Graphene has high mobility at room temperature

[1] Zhu et al. "Graphene geometric diodes for terahertz rectennas." *Journal of Physics D: Applied Physics* 46.18 (2013): 185101.
[2] Auton et al. "Terahertz detection and imaging using graphene ballistic rectifiers." *Nano letters* 17.11 (2017): 7015-7020.

Introduction: Simulation strategy

Dimensions are important

Device's dimensions:

≈ nm

- Quantum transport simulations
- NEGF/DFT/Scattering matrix method

Device's dimensions:

nm-µm

- Semi-classical transport
- Monte Carlo Simulations

Device's dimensions:

> µm

- classical transport
- Drift-diffusion model

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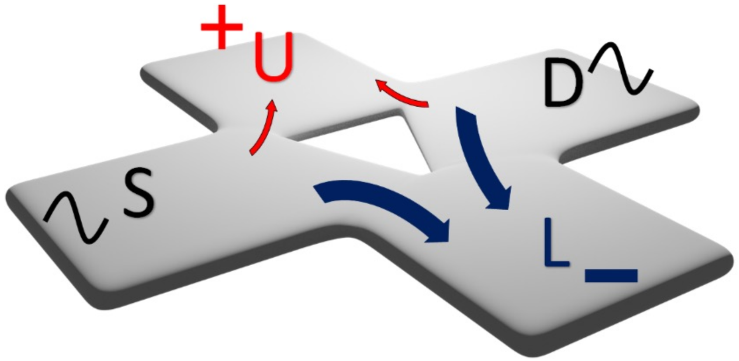
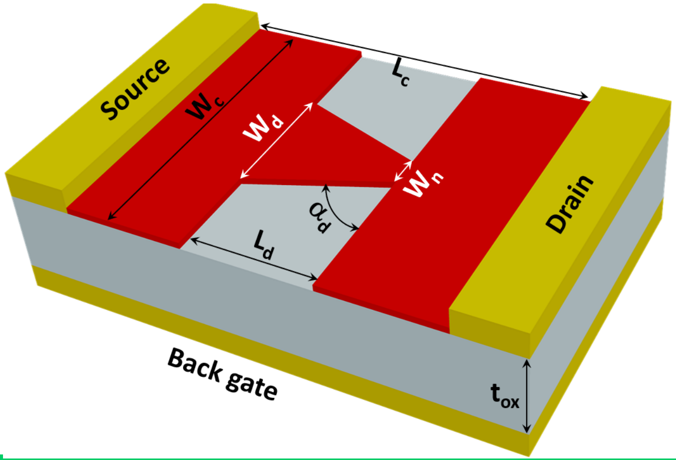
Model: Simulated structures





1. **Mixed model Landauer-Buttiker and Monte Carlo**
   - Uniform electric field regime (No electrostatics effects)
   - Mixed carrier transport
   - Ballistic and scattering regime

4. **Self-consistent simulation**

2. **Uniform electric field regime (No self-consistency with Poisson equation)**
   - Ballistic regime & only electron transport
3. **Self-consistent simulation (all the electrostatics effects are taken into account)**
   1) Ballistic regime & only electron transport
   2) Time domain simulation
   3) Mixed carried transport
   4) Scattering effects due to intrinsic and remote phonons, grain boundary and defects

Model: MC Landauer-Buttiker model

Synergistic use of Monte Carlo Simulation and Landauer-Buttiker formalism

Imposing $I_L = I_U = 0$ we find

$$\boldsymbol{V_{LU}} = \frac{\boldsymbol{G_{LS}(V_{SD})G_{UD}(V_{SD}) - G_{LD}(V_{SD})G_{US}(V_{SD})}}{\boldsymbol{G_L S - \left(G_{SL}(V_{SD}) + G_{DL}(V_{SD})\right)\left(G_{LD}(V_{SD}) + G_{LS}(V_{SD})\right)}}\boldsymbol{V_{SD}} = \frac{\boldsymbol{A(V_{SD})}}{\boldsymbol{B(V_{SD})}}\boldsymbol{V_{SD}}$$

$$\boldsymbol{G_{ij}(n, V_{SD}) = G_{ij}{}^{e}(n, V_{SD}) + G_{ij}{}^{h}(p, V_{SD})}$$

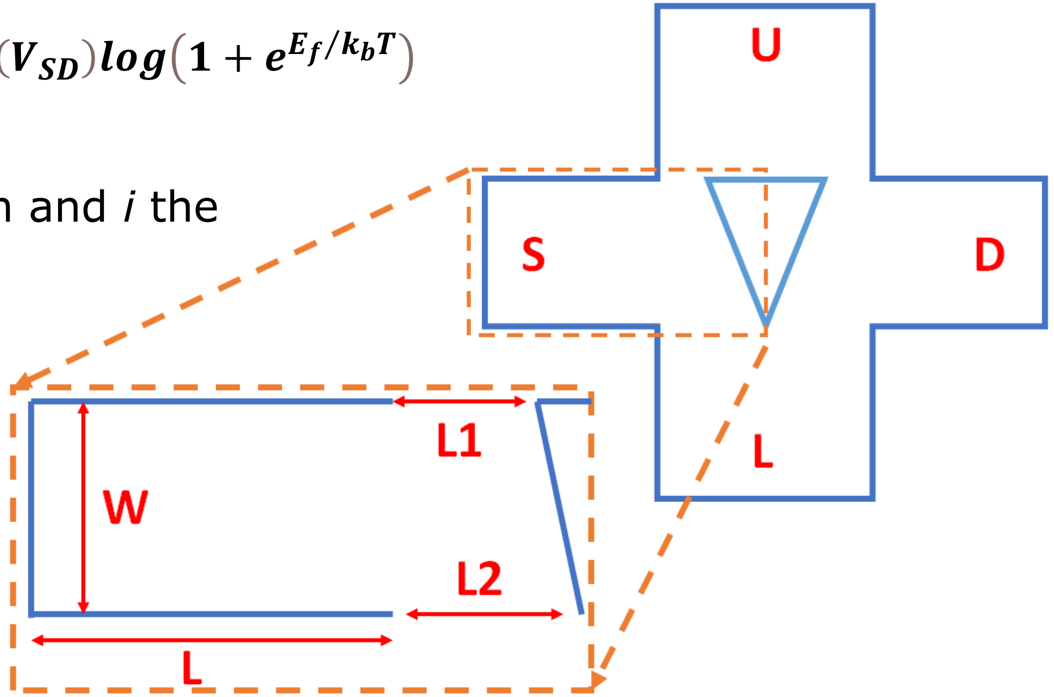
$$\boldsymbol{G_{ij}^{e/h}(V_{SD}) = \frac{2q^2 W k_b T}{\pi^2 v_f \hbar^2} T_{ij}(V_{SD}) log\left(1 + e^{E_f/k_b T}\right)}$$

T_{ij} is the transmission probability $0 \le T_{ij} \le 1$ where j is the injection and i the collection terminal

T_{ij} calculated with MC simulator

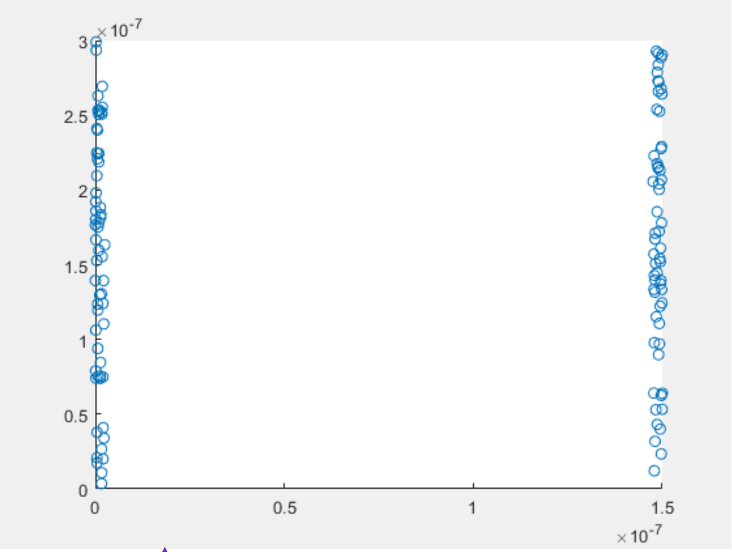
Thanks to symmetry conditions we can restrict simulations to a sub-region of the overall device

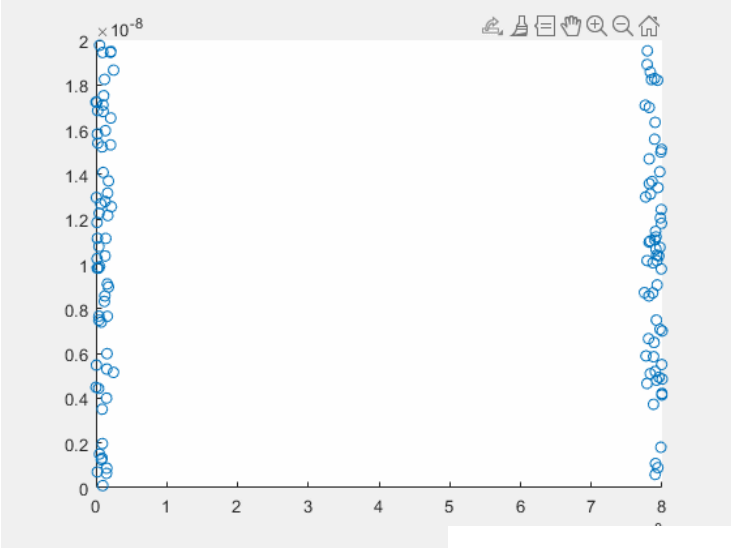
For $I_L = I_U = 0$ $\boldsymbol{T_{ij} = T_{ji}}$ with $j \neq \{S, D\}$



Song A., Physical review B 59.15 (1999): 9806.
Truccolo et al. *Solid-State Electronics* 194 (2022): 108314.

Model:Monte Carlo/ Poisson scheme



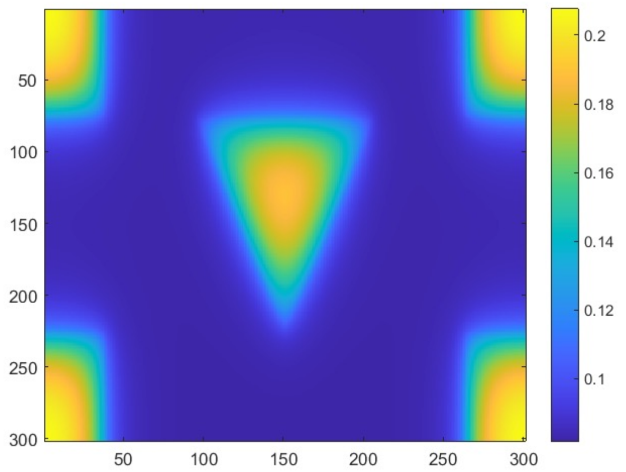


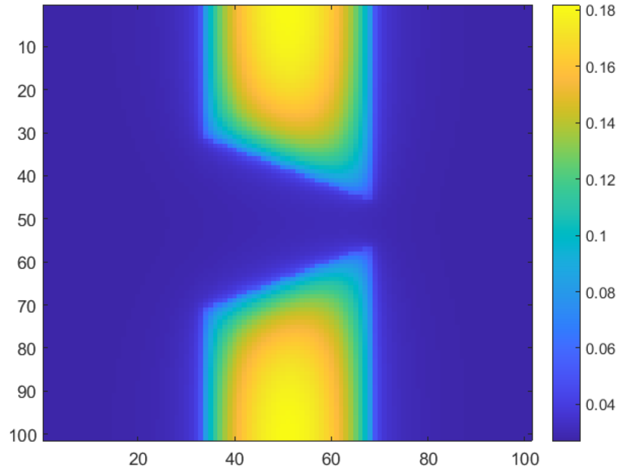
Charge motion according to semiclassical equation

$$\begin{cases} \varepsilon(\vec{k}) = \hbar v_f |\vec{k}| \\ \hbar \dot{\vec{k}} = -q\vec{E}(r) \\ \dot{\vec{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} = v_f \frac{\vec{k}(t)|}{|\vec{k}(t)|} \end{cases}$$

Non-linear 3D Poisson equation

$$\nabla\left(\varepsilon \nabla \varphi^{(k+1)}\right) = \delta(z) n^{(k)}\, e^{\frac{q(\varphi^{(k+1)} - \varphi^{(k)})}{k_b T}}$$





IEEE SSCS Electron Devices Society GreEnergy

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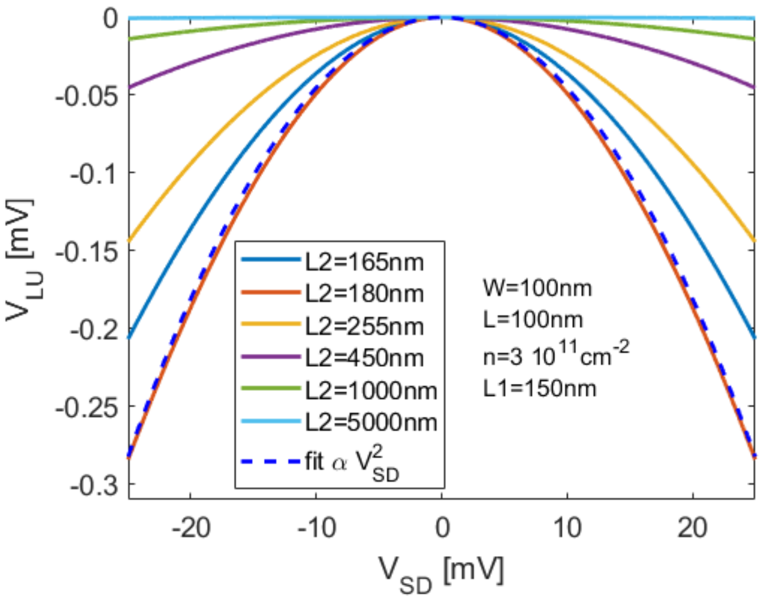
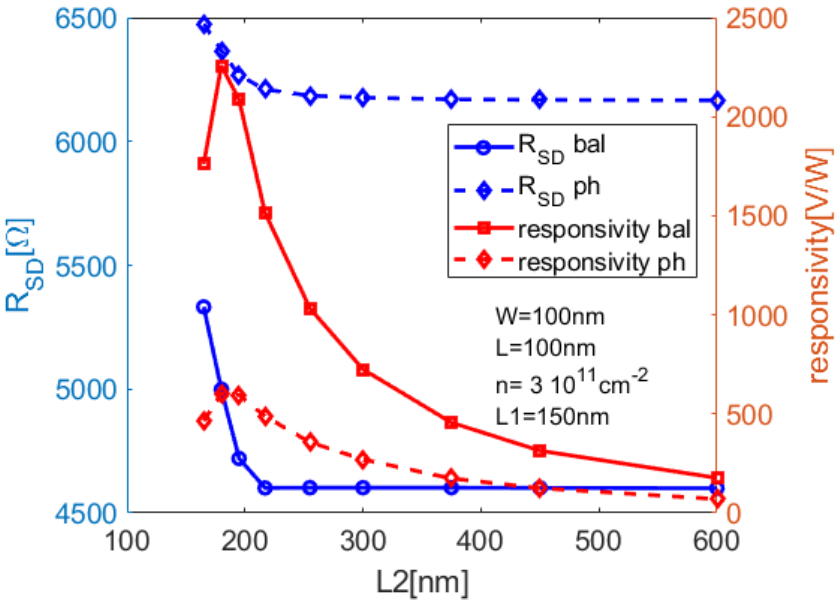
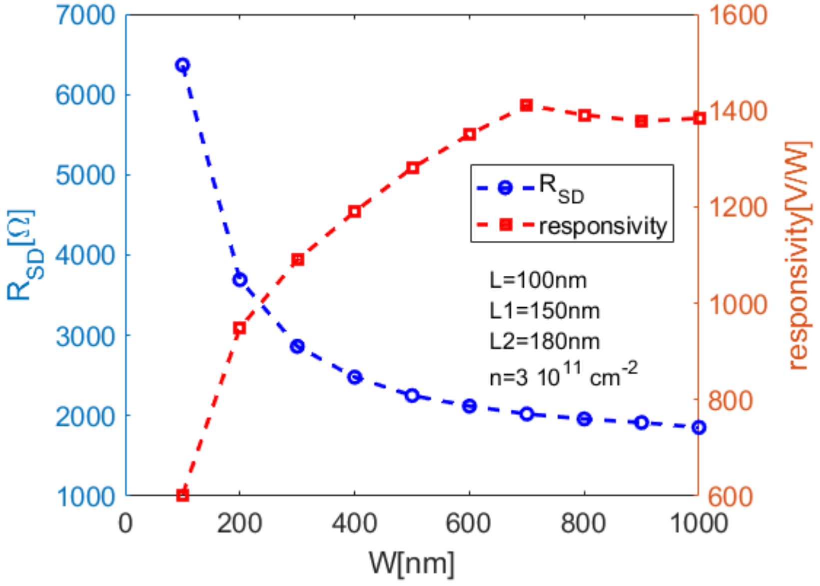
Results: 4-terminal device



(ballistic regime)

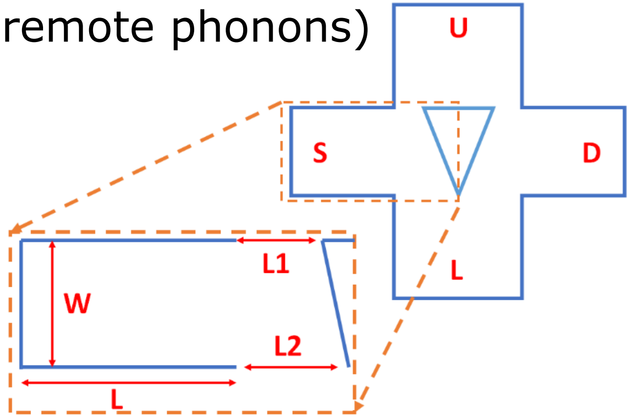


(ballistic & int.+remote phonons)



(int.+remote phonons)

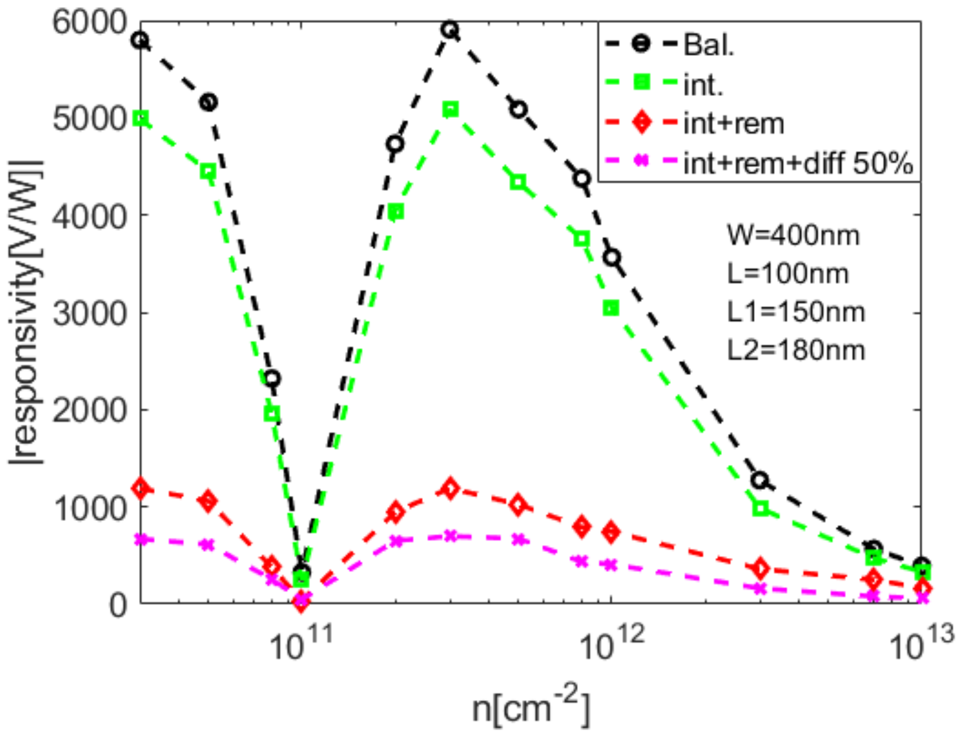
$$responsivity = \lim_{V_{DS}\to 0} \frac{V_{LU}}{P_{input}}$$

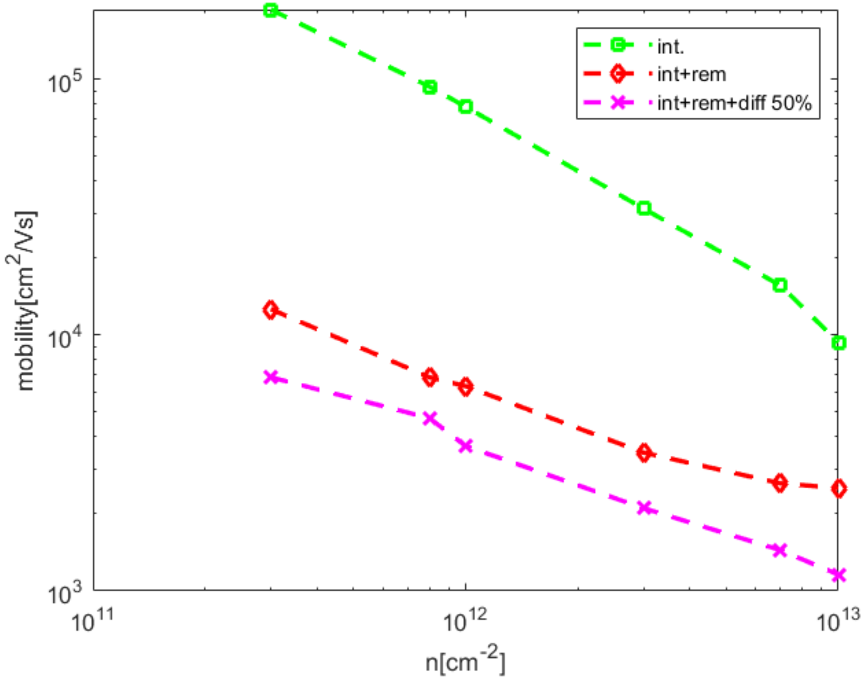


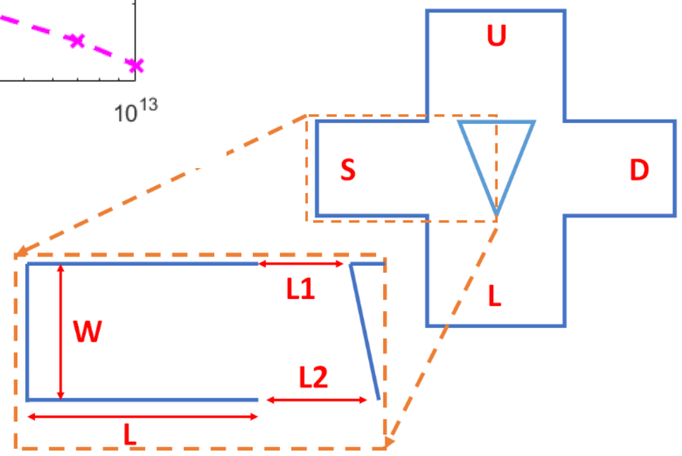
- Device characterization as a function of geometrical parameters

Truccolo et al. *Solid-State Electronics* 194 (2022): 108314.

Results: 4-terminal device







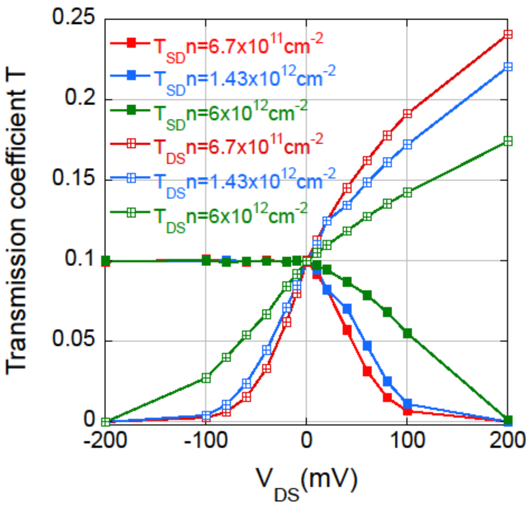
- Device performance for different transport condition

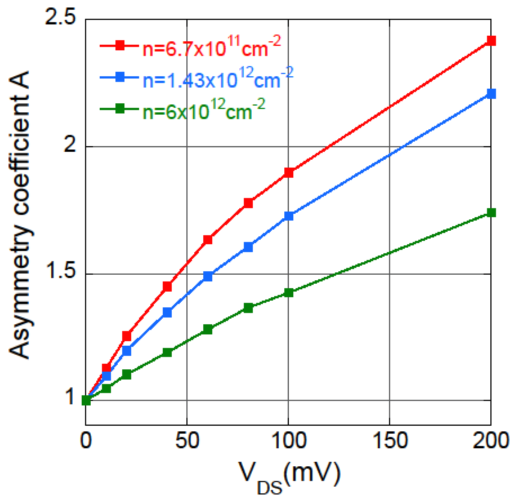
Truccolo et al. *Solid-State Electronics* 194 (2022): 108314.

Results: 2-terminal device

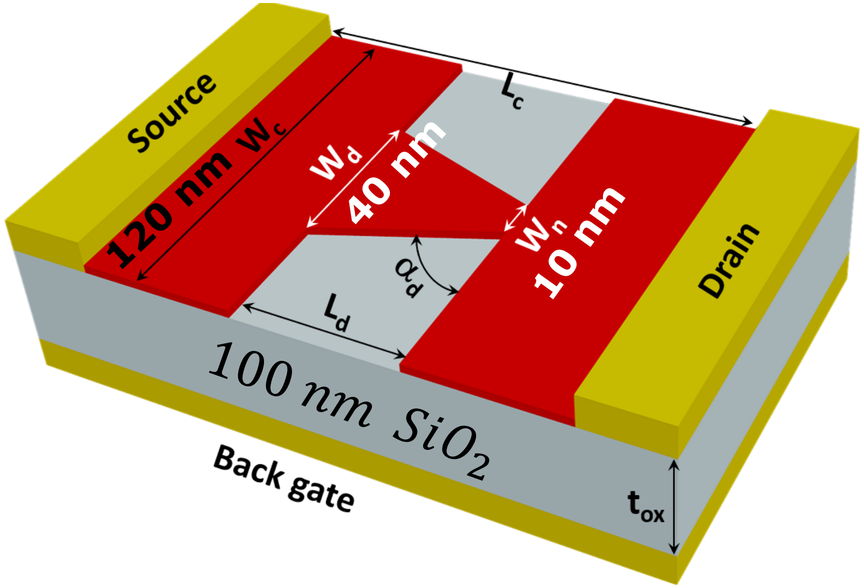
Uniform electric field regime

$$A \approx \frac{T_{DS(+V_{DS})}}{T_{SD(-V_{DS})}}$$



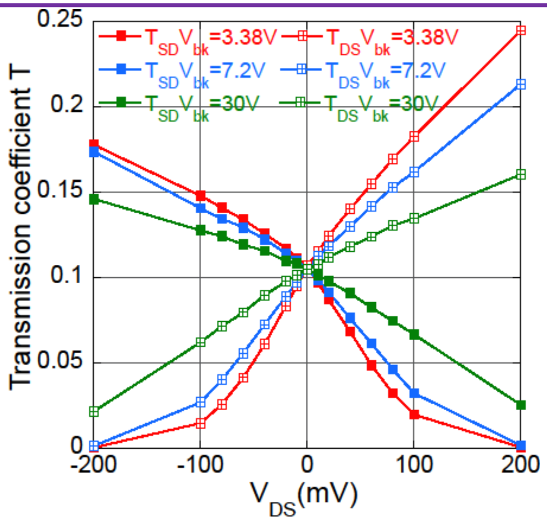


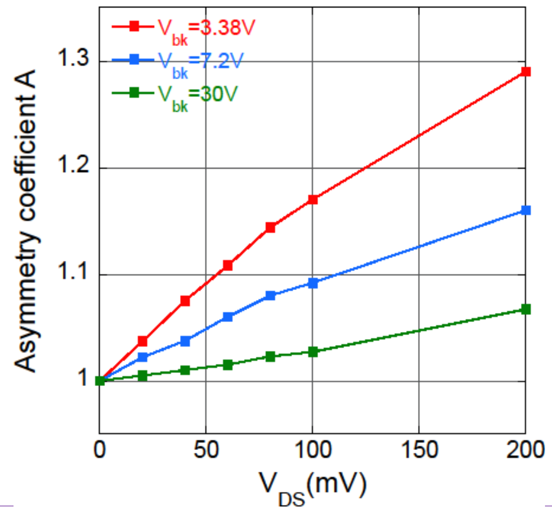
- Higher gate voltage induces higher electron density on Gr
- The Fermi wave vector on Gr is $k_f = \sqrt{2\pi n}$
- More electric field E_x needed to align the injected electrons into the device
- **Reduction of asymmetry**



Self-consistent regime

$$A = \frac{I_{DS(+V_{DS})}}{I_{SD(-V_{DS})}}$$



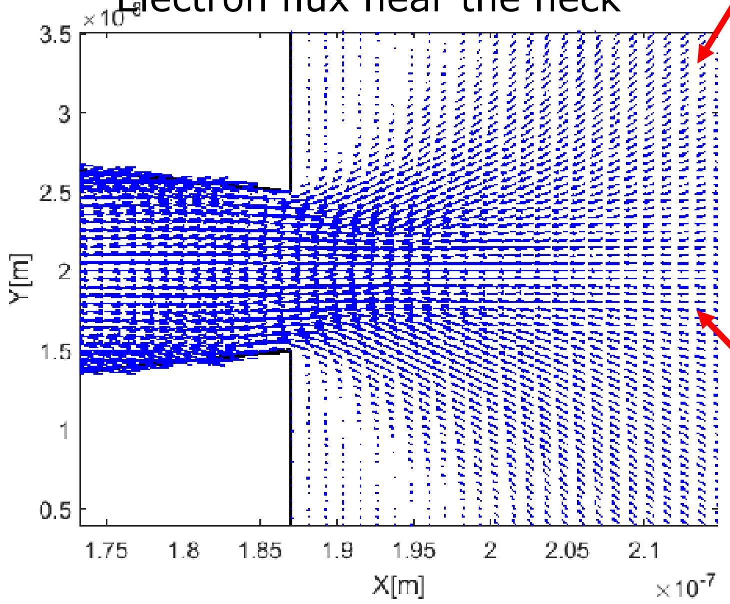


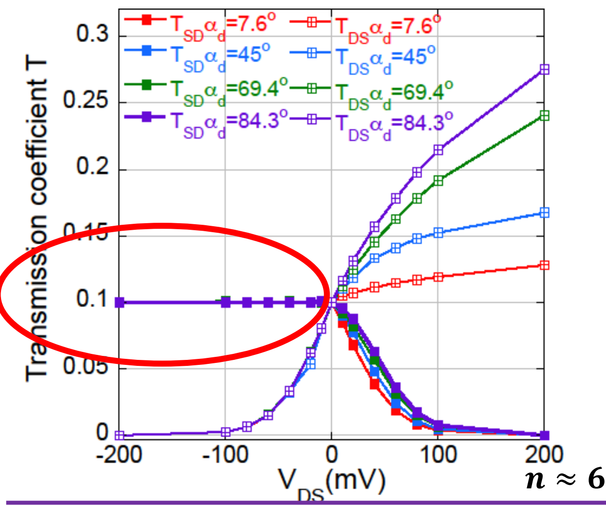
Truccolo et al. ,IEEE TED, vol. 71, no. 2, pp. 1294-1301

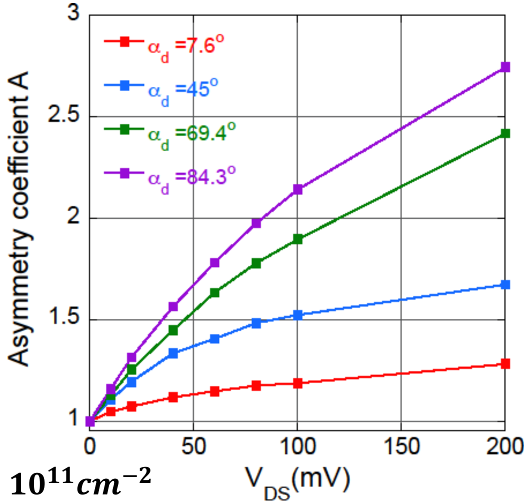
Results: 2-terminal device

- The electrostatics effects in proximity of the neck cause an extra electrons injection from Drain to Source terminals
- **Reduction of asymmetry**

Electron flux near the neck

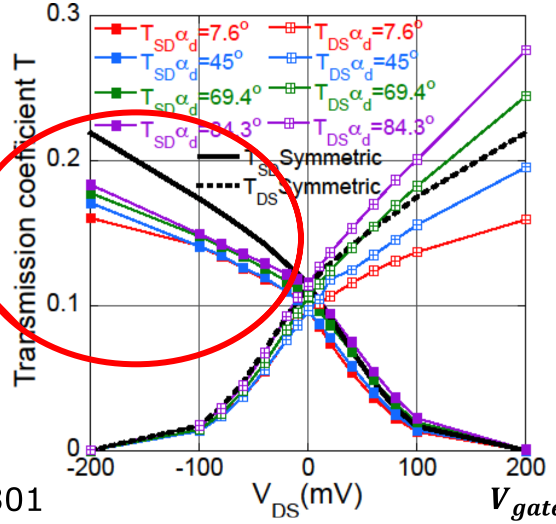


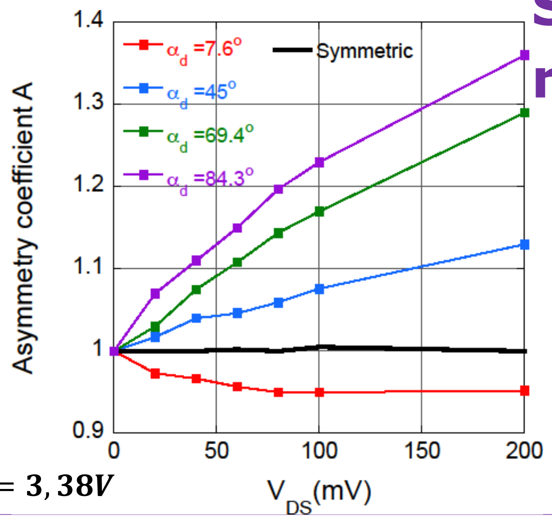




$n \approx 6,7\ 10^{11} cm^{-2}$

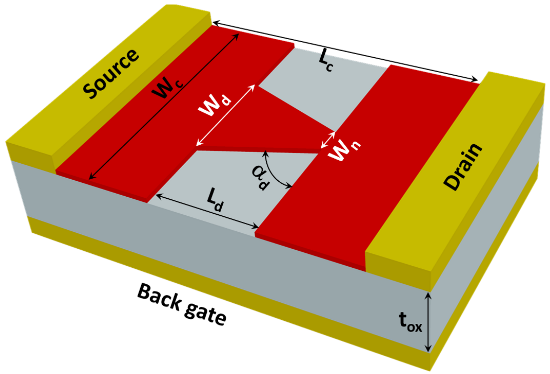
Uniform electric field regime





$V_{gate} = 3,38V$

Self-consistent regime



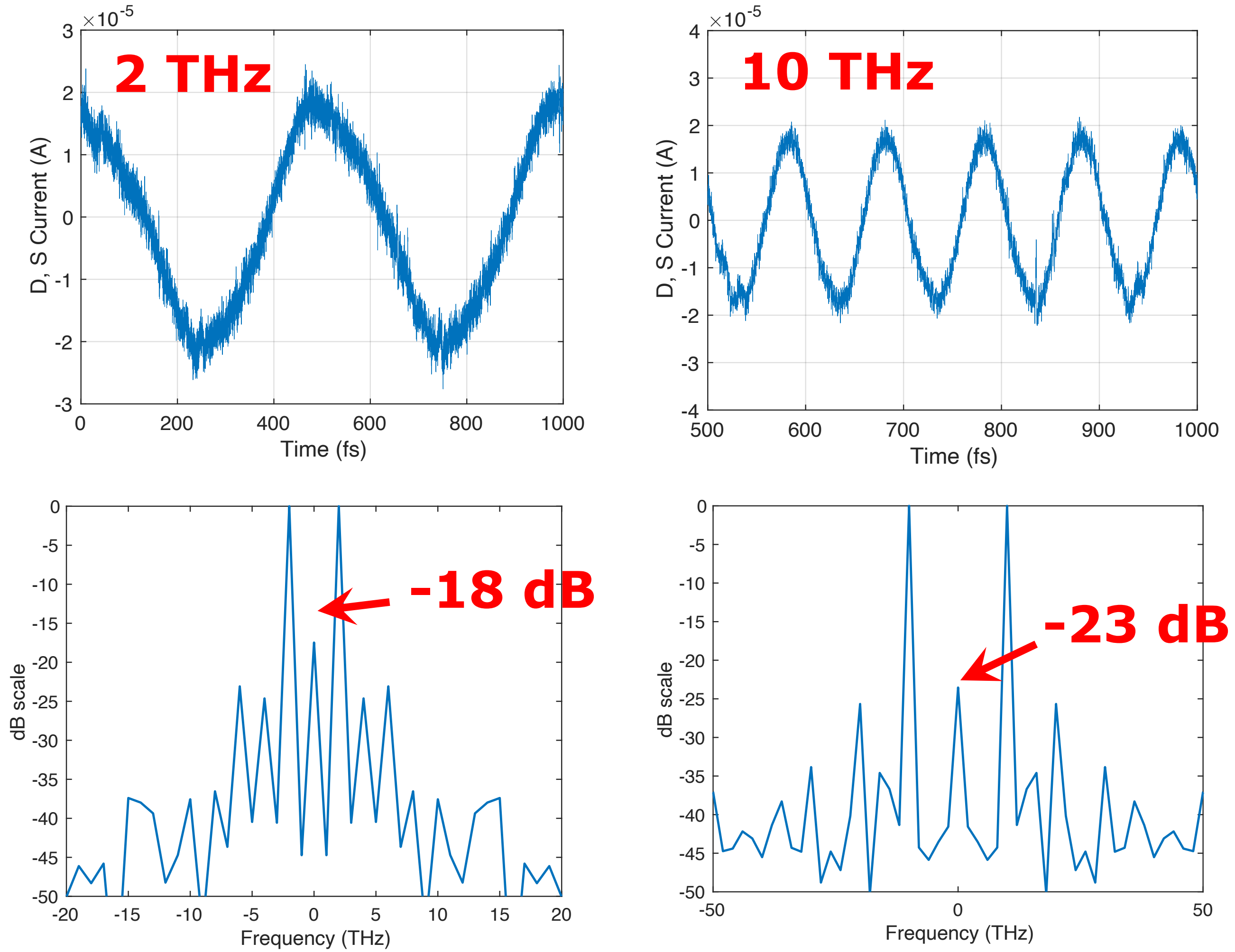
Truccolo et al. ,IEEE TED, vol. 71, no. 2, pp. 1294-1301

Results: 2-terminal time domain

$$\nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = -\mu \vec{J}_i$$

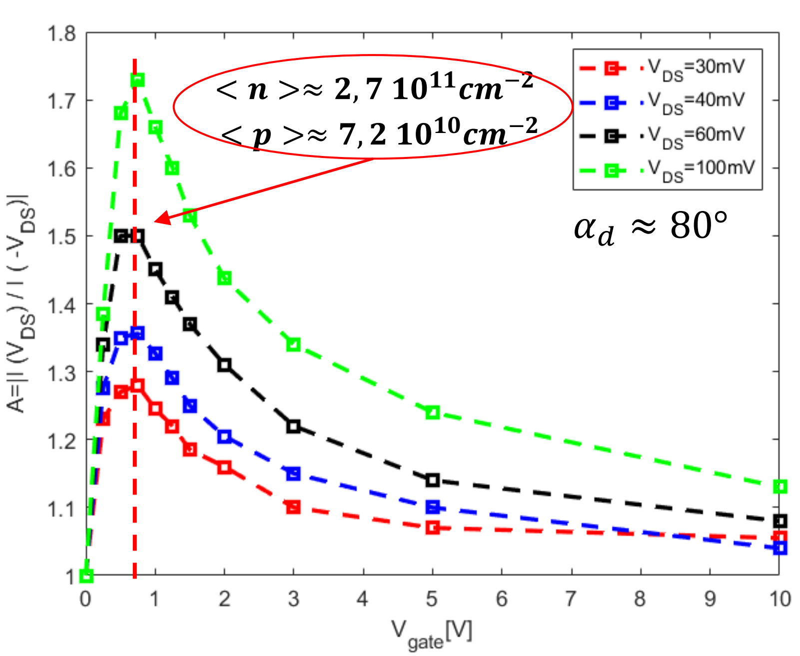
$$\nabla^2 \varphi - \frac{1}{c^2}\frac{\partial^2 \varphi}{\partial t^2} = -\rho/\epsilon$$

Poisson / Maxwell eq.

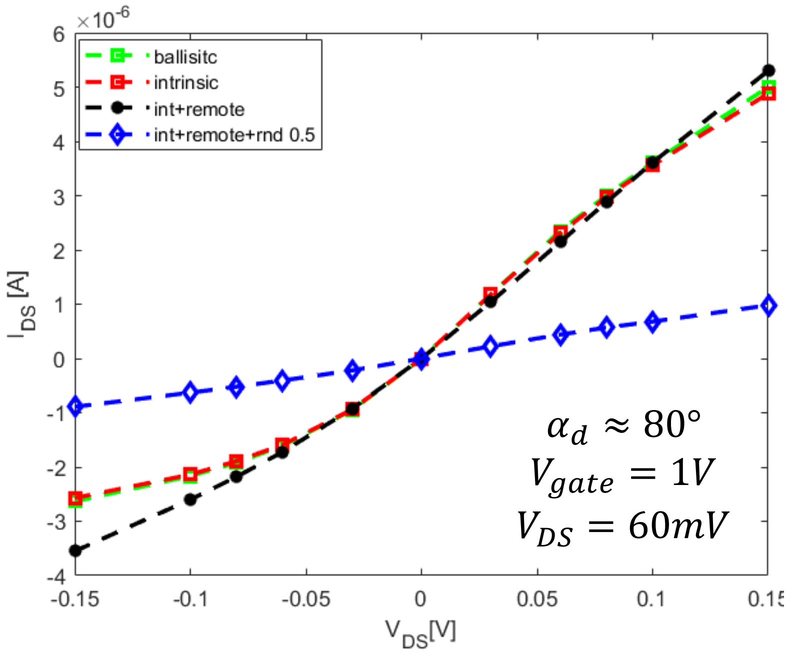


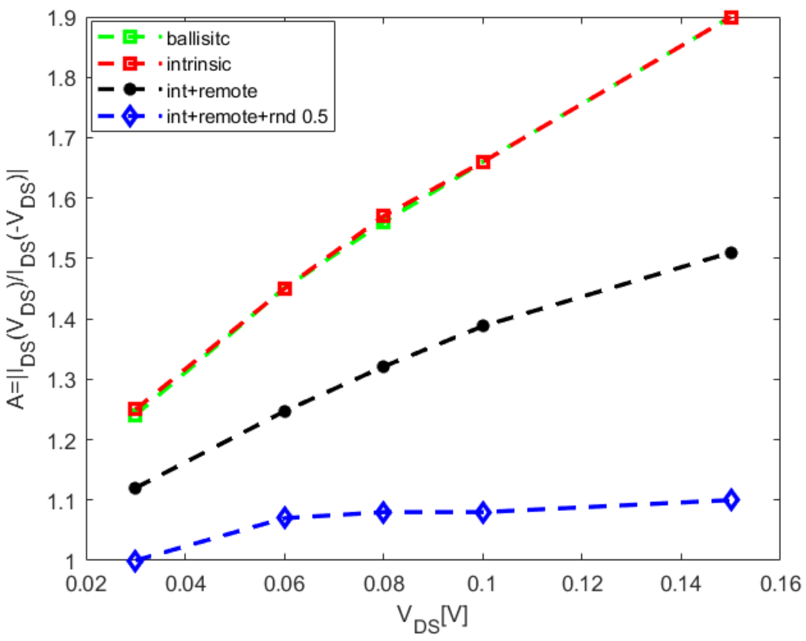
- **Device frequency limit?**
- **Limit of semi-classical time domain analysis**
- **Photon-electron interaction must be taken into account !**

Results: Mixed transport & effects of scattering in 2-terminal device



(mixed transport in ballistic regime)

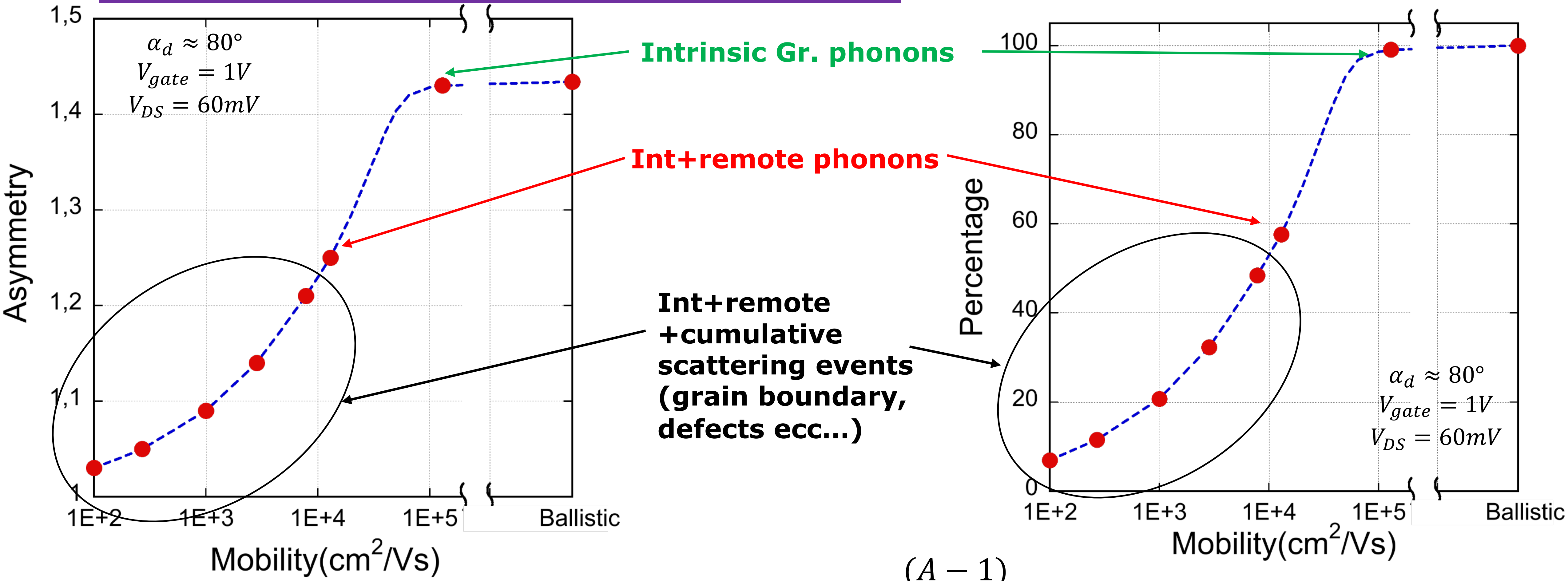




(mixed transport with int.+remote phonons + random scattering)

Truccolo et al. under publication

Results: Effects of scattering in 2-terminal device



$$Percentage = \frac{(A-1)}{(A_{max}-1)}$$

Truccolo et al. under publication

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Conclusion: Overview

- **progressive complexity of the simulations**

  I. MC uniform electric field simulations & Landauer-Buttiker formalism
  II. Self-consistent MC simulation (only ballistic)
  III. Self-consistent MC simulations with different scattering mechanisms

- **Time domain simulations**

  I. Limit of the semi-classical time domain analysis

- **Future goals**

  I. Self-consistent simulation for the 4-terminal device with different transport condition
  II. Inclusion of electron/photon interaction

Thank you!

GreEnergy
Power from optical antennas

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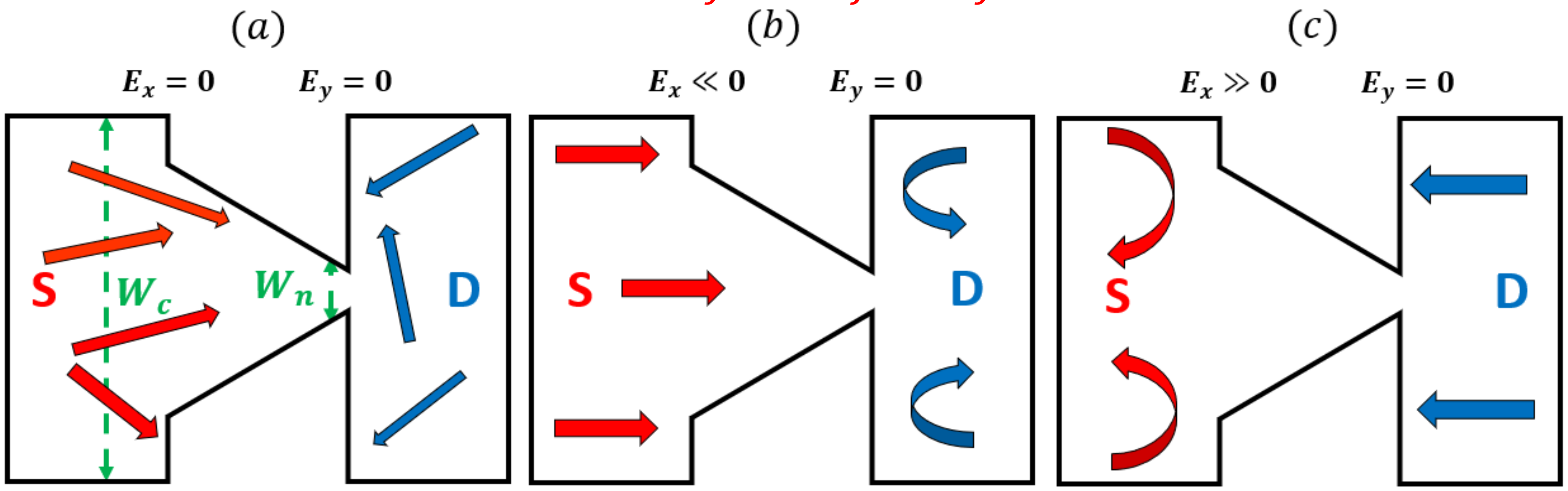
Backup slides

Uniform electric field regime: working principle

Uniform electric field: $E_x = -\frac{V_{DS}}{L_c}$ $E_y = 0$

$$T_{ij} = \frac{n\ electrons\ pass\ through\ i}{total\ electrons\ injected\ from\ j}$$



(a) $T_{DS} = T_{SD} = \frac{W_n}{W_c}$

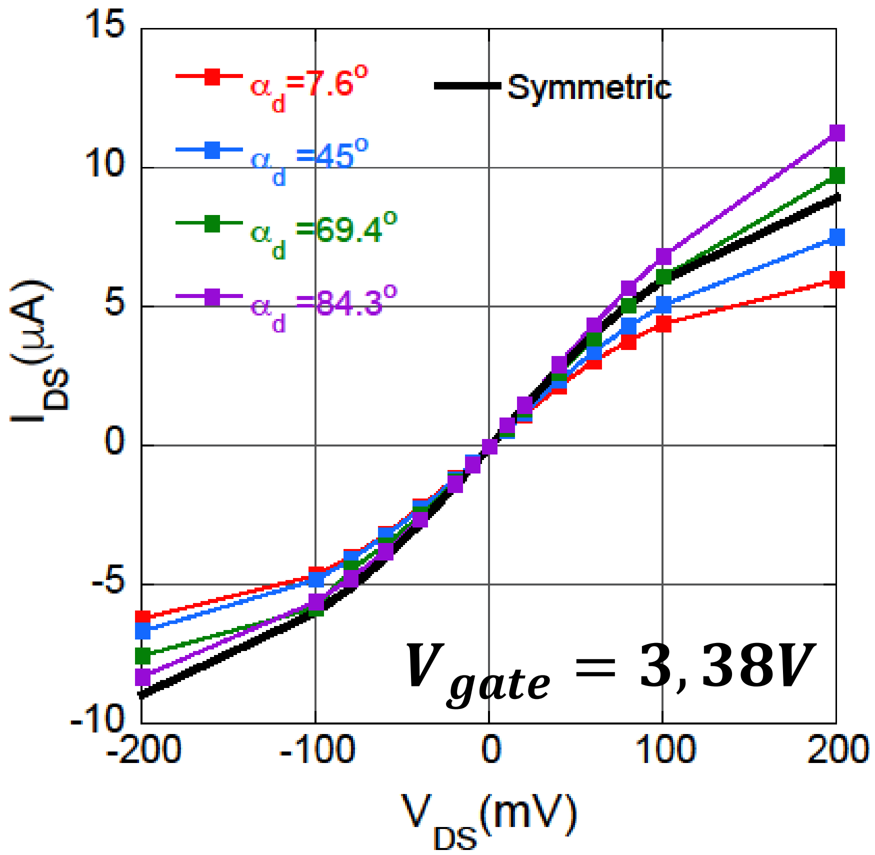
(b) $T_{DS} > \frac{W_n}{W_c}$

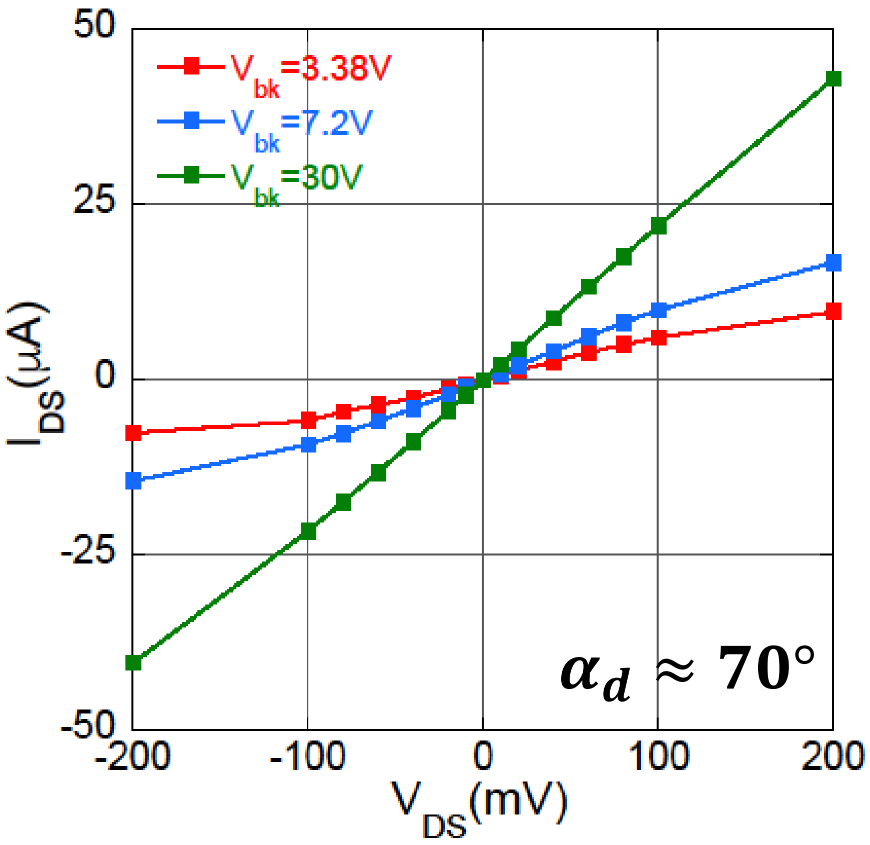
$T_{SD} \to 0$

(c) $T_{DS} \to 0$

$T_{SD} = \frac{W_n}{W_c}$

Self-consistent simulation: I-V 2-terminal





FDTD stability

$$\Delta t < \frac{\Delta r}{c}$$

Courant's limit

Spatial step

time step

$\Delta r \approx 1nm$ **(mesh dimensions)** → $\Delta t \approx 10^{-18}s$

@ 1 THz 1period $= 10^{-12}$s → 10^{6}step

@ 1 GHz 1period $= 10^{-9}$s → 10^{9}step

→ Every step each mesh pixel must be filled with particles (well defined density matrix) → high computation time