On the Role of Line-Edge Roughness on the Diffusion and Localization in GNRs

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Outline

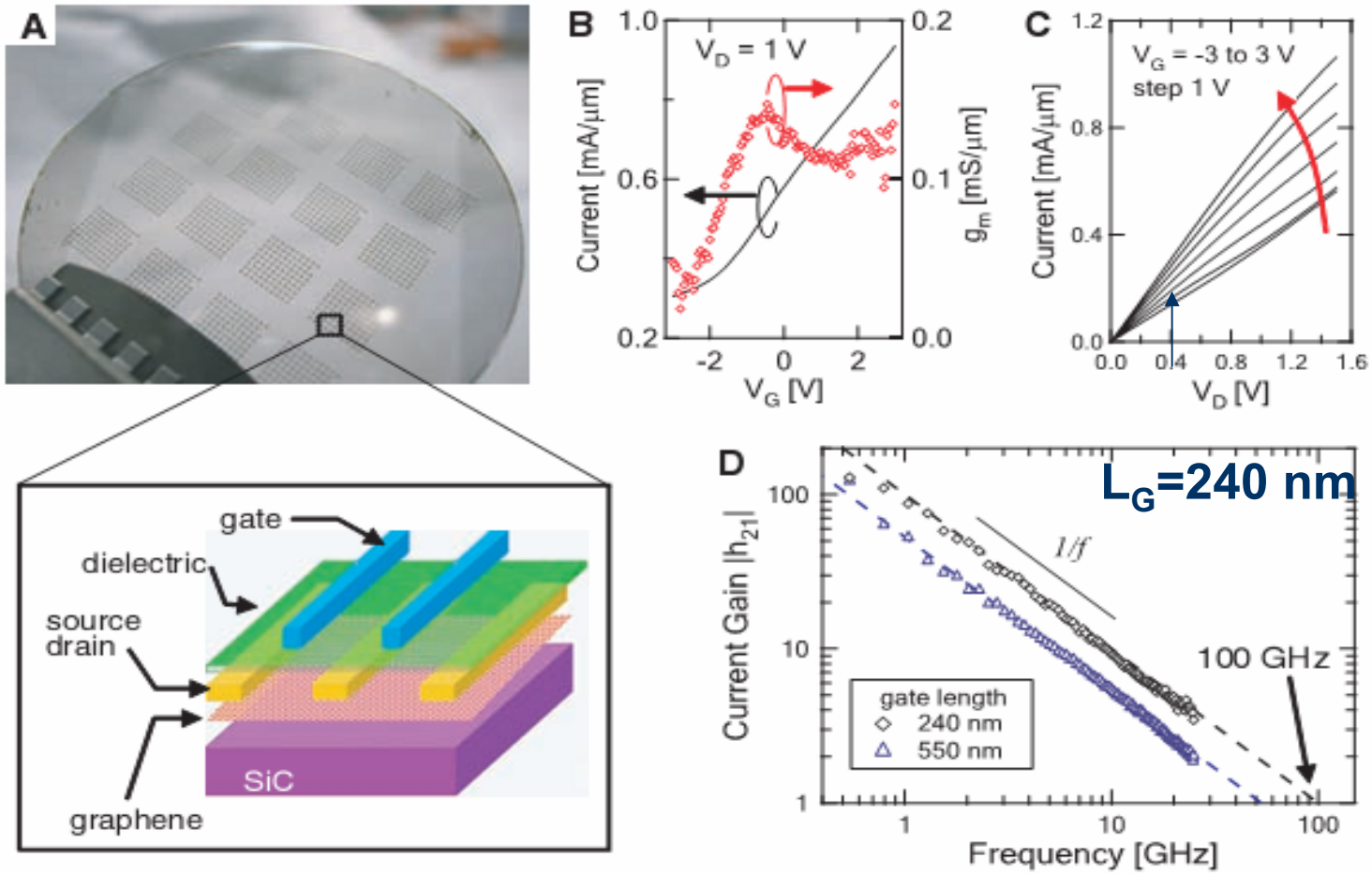
- Introduction
- Modeling of line-edge roughness
- Line-edge roughness in graphene nanoribbons (GNRs)
- Diffusive transport regime
- Localization regime
- Conclusions

Why Carbon Based Electronics?

- Semiconducting GNRs can be used as transistor channels
- Metallic GNRs can be used as interconnect lines
- High electronic conductivity, quasi-ballistic transport
- High thermal conductivity
- Symmetric dispersion relation for electrons and holes
- Direct and narrow band-gap: Optoelectronic applications

Carbon Based Electronics

- **Graphene based transistor with f_T=100 GHz (IBM 2010)**

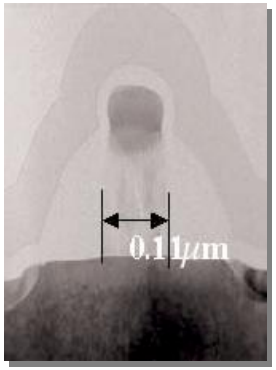


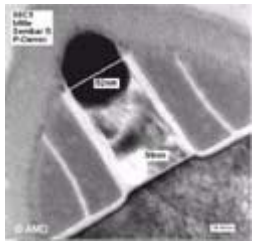
Lin, Science. 327, p.622 (2010)

Introduction

- **Hierarchy of semi-classical and quantum transport models**

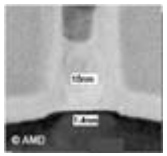
Transport regime	Semi-classical $L > \lambda_e$				Quantum mechanical $L \sim \lambda_e$	
Fundamental equation	Boltzmann equation				Schrödinger equation	
Transport model	Drift-diffusion	Hydrodynamic	Boltzmann	Quantum corrected Boltzmann, Quantum hydrodynamic	Density matrix, Wigner eq	Non-equilibrium Green's function



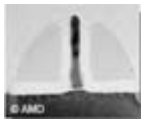


90nm Generation

45nm Generation



32nm Generation



22nm Generation

Introduction

- **Ballistic transport:** L < λ

$$G = G_0 N_{\mathrm{ch}}$$

- **Diffusive transport:** λ < L < ξ

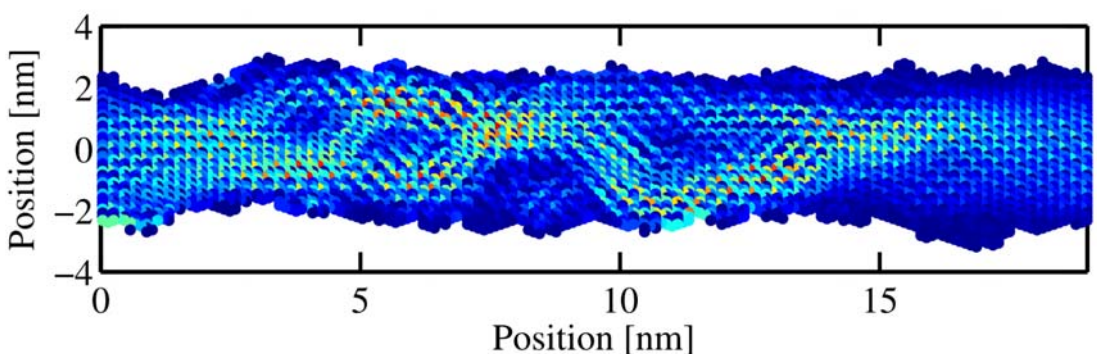
$$G = \frac{G_0 N_{\mathrm{ch}}}{1 + L/\lambda}$$

- **Localization regime:** λ < ξ < L

$$\langle \ln \{G/G_0\} \rangle \propto -L/\xi$$

$$G_0 = \frac{2q^2}{\hbar}$$

  - $N_{ch}(E)$ … number of conducting channels at energy E
  - λ …mean free path
  - ξ ... localization length



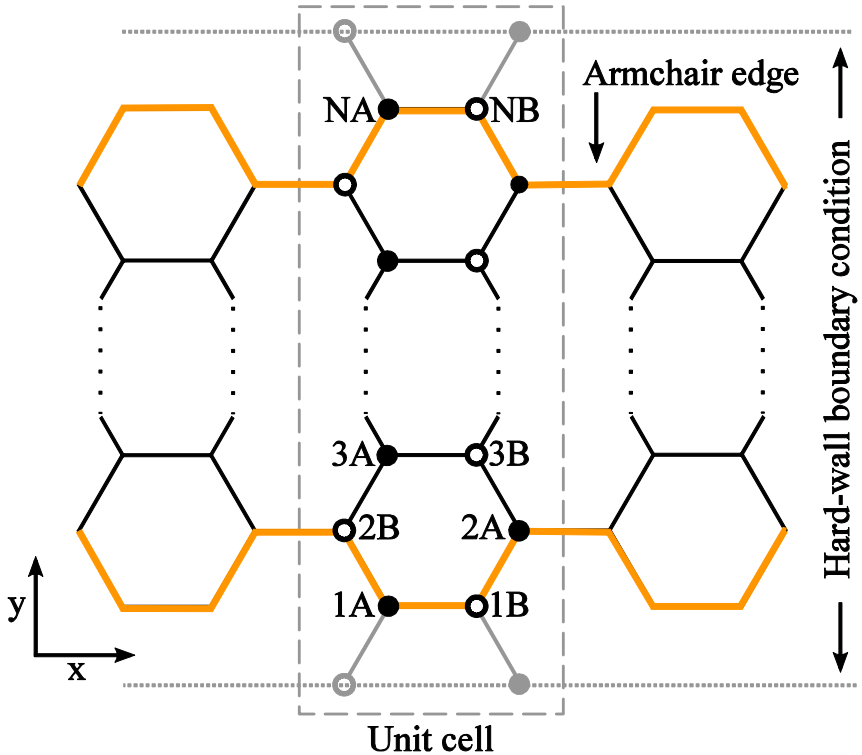
Non-Equilibrium Green's Function Formalism

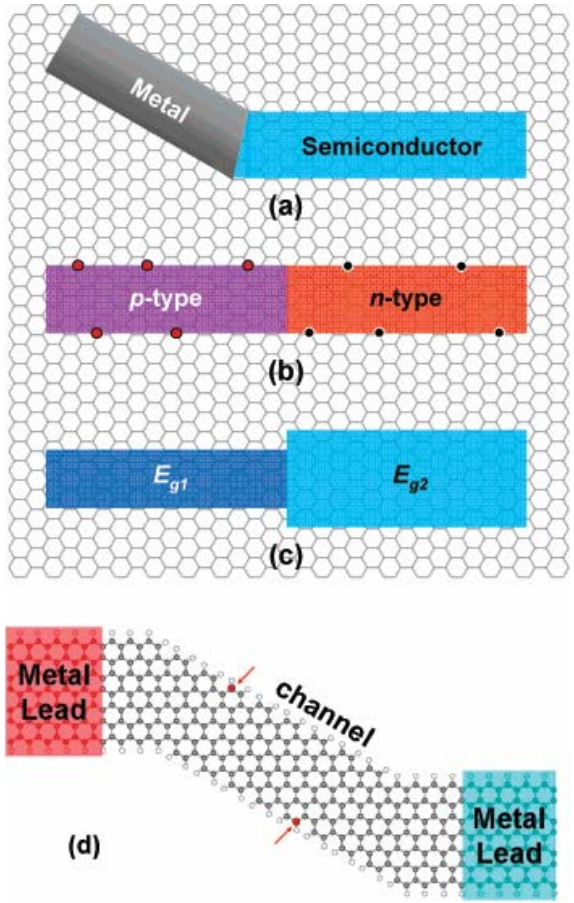
- Open systems (contacts)
- Non-equilibrium (electric field, optical excitation)
- Quantum transport (tunneling)
- Interaction effects (scattering)

Non-Equilibrium Green's Function formalism (NEGF)

- Foundations: The NEGF technique emerged from the Schwinger school in the early 60's and work on non-equilibrium quantum statistical mechanics by Kadanoff-Baym (1962) and Keldysh (1965)
- Application: Caroli (1971) appeared to be the first who applied this technique to calculate current through a device

Graphene Nano-Ribbons





Yan, et al. , Nano Lett. 7, p.1469, 2007

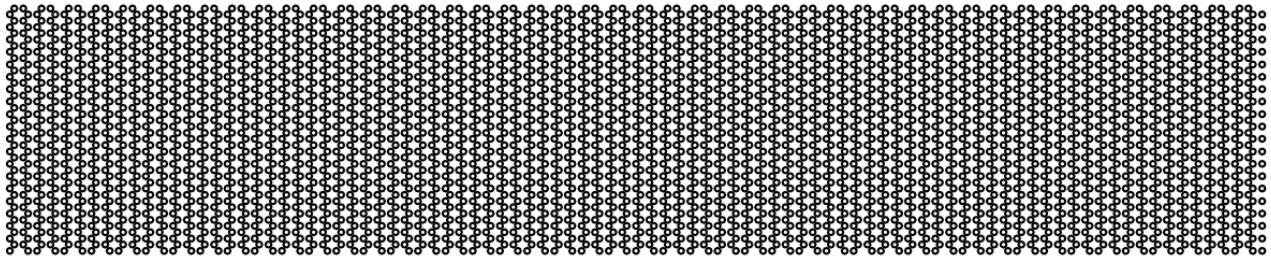
Line-Edge Roughness in GNRs

- **Line-edge roughness in GNRs**
- **Exponential model for roughness autocorrelation c(n)**

$$c(n) = \Delta_m^2 \exp\left(-\frac{x}{L_m}\right), \quad x = n\Delta x$$

  - Roughness amplitude (Δ_m)
  - Correlation length (L_m)

Δ_m = 0.00 nm (Perfect GNR)



S.M. Goodnick, Phys. Rev. B 32, p.8171 (1985)

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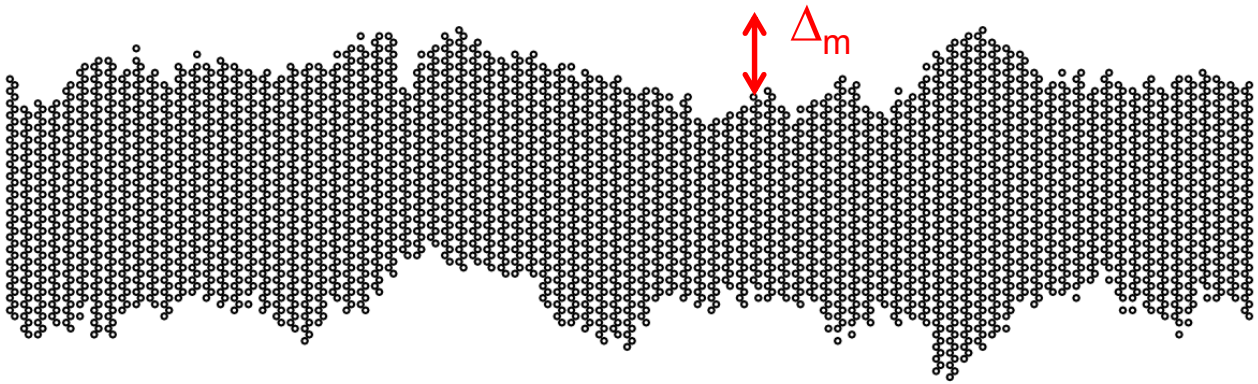
Δ_m = 0.50 nm ↑ L_m = 3.00 nm



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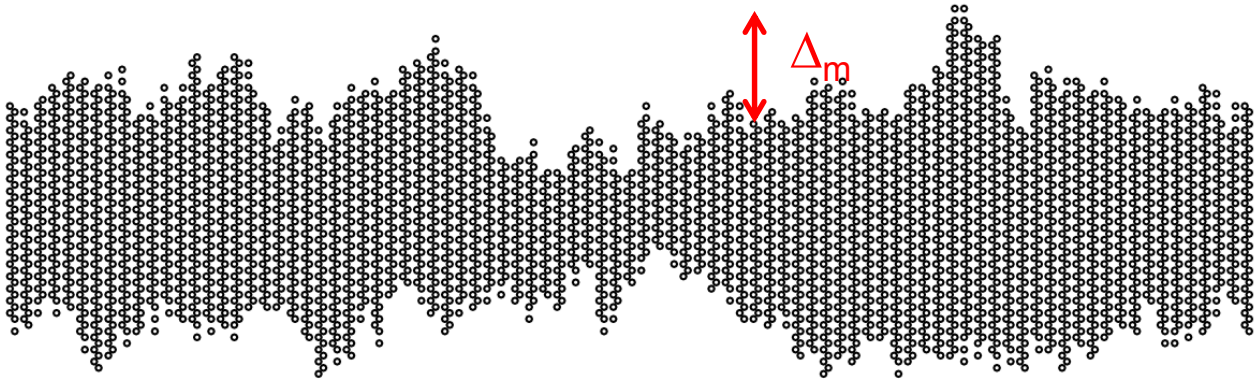
Δ_m = 0.75 nm ↑ L_m = 3.00 nm



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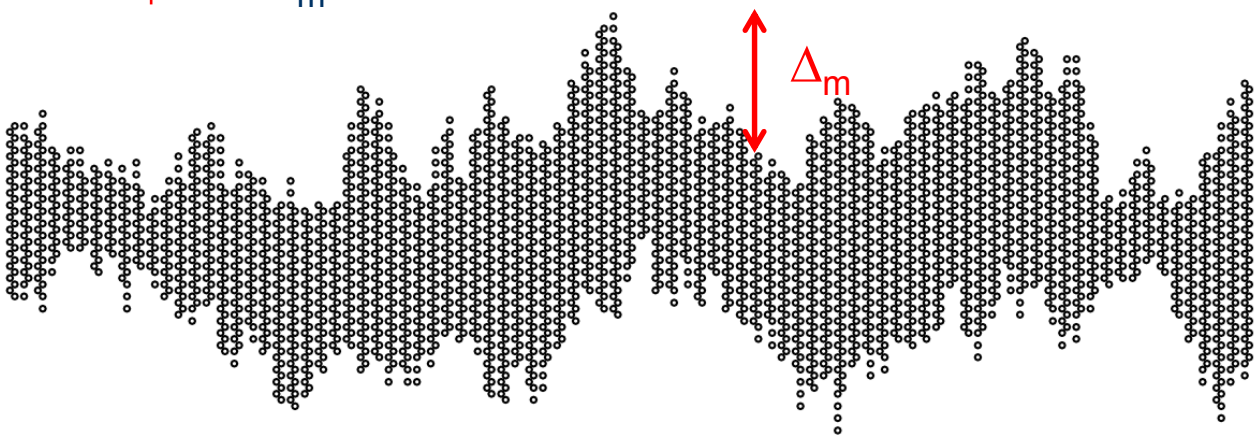
Δ_m = 1.00 nm ↑ L_m = 3.00 nm



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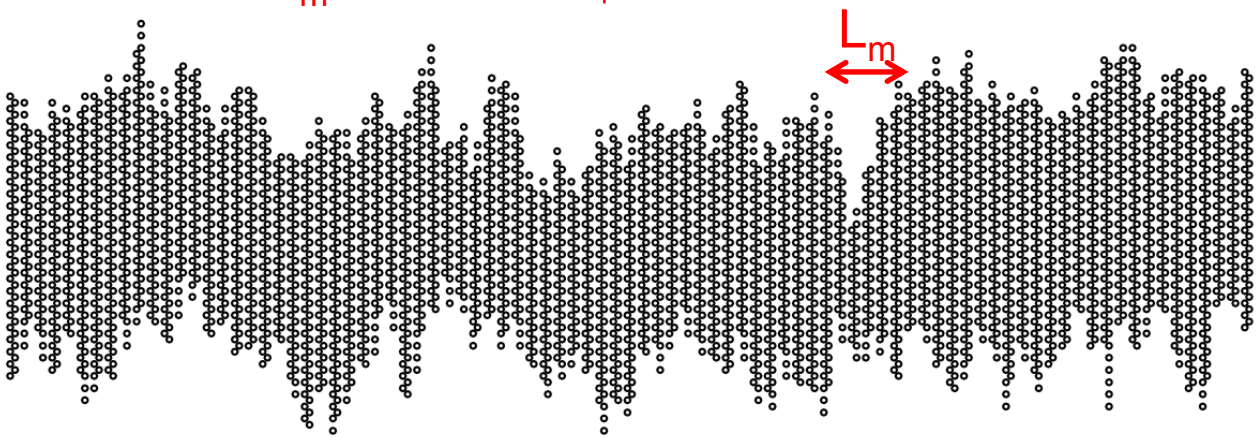

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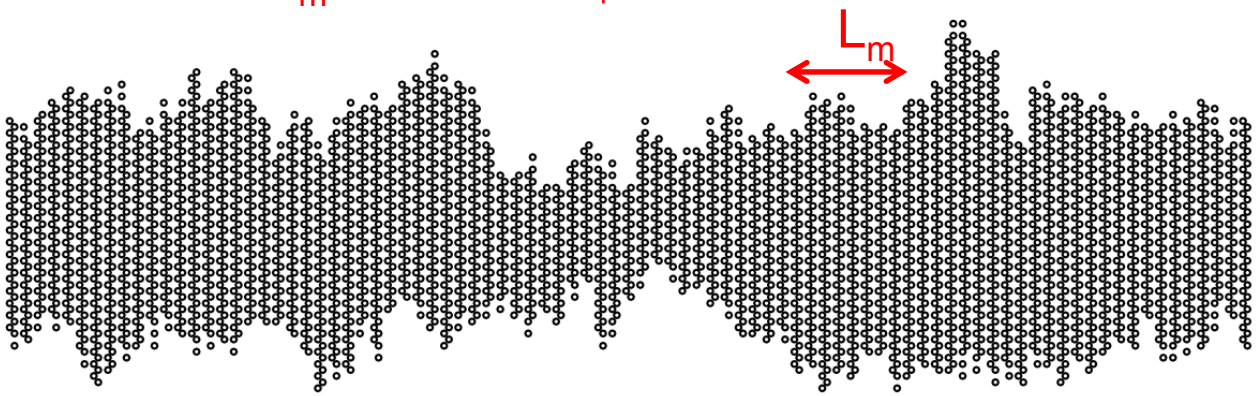

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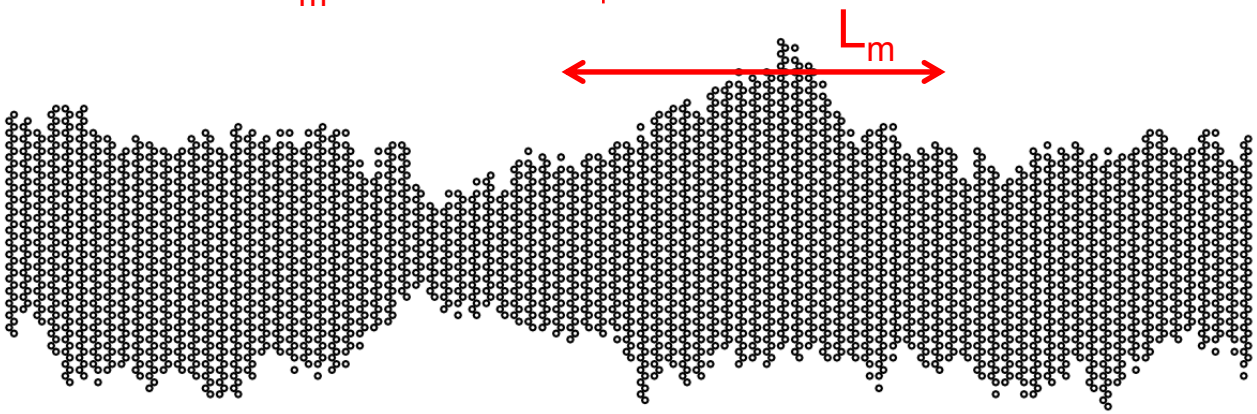
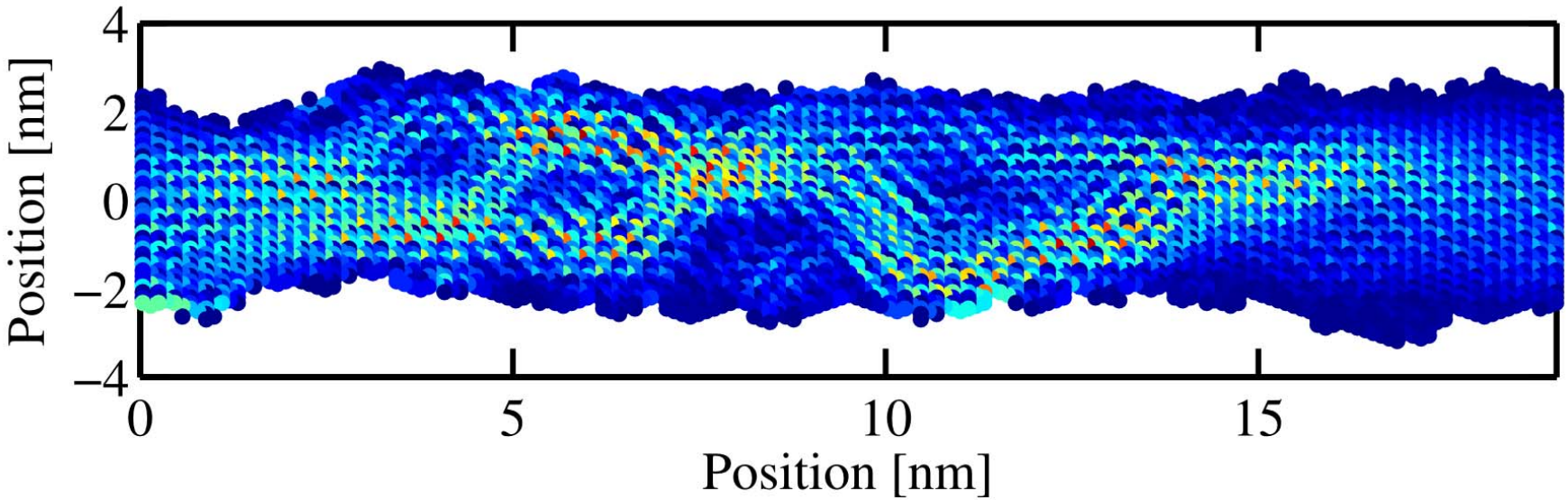
Δ_m = 0.75 nm L_m = 6.00 nm ↑



Line-Edge Roughness in GNRs

- **Line-edge roughness in GNRs**
- **Current spectrum**

Δ_m = 0.50 nm L_m = 3.00 nm



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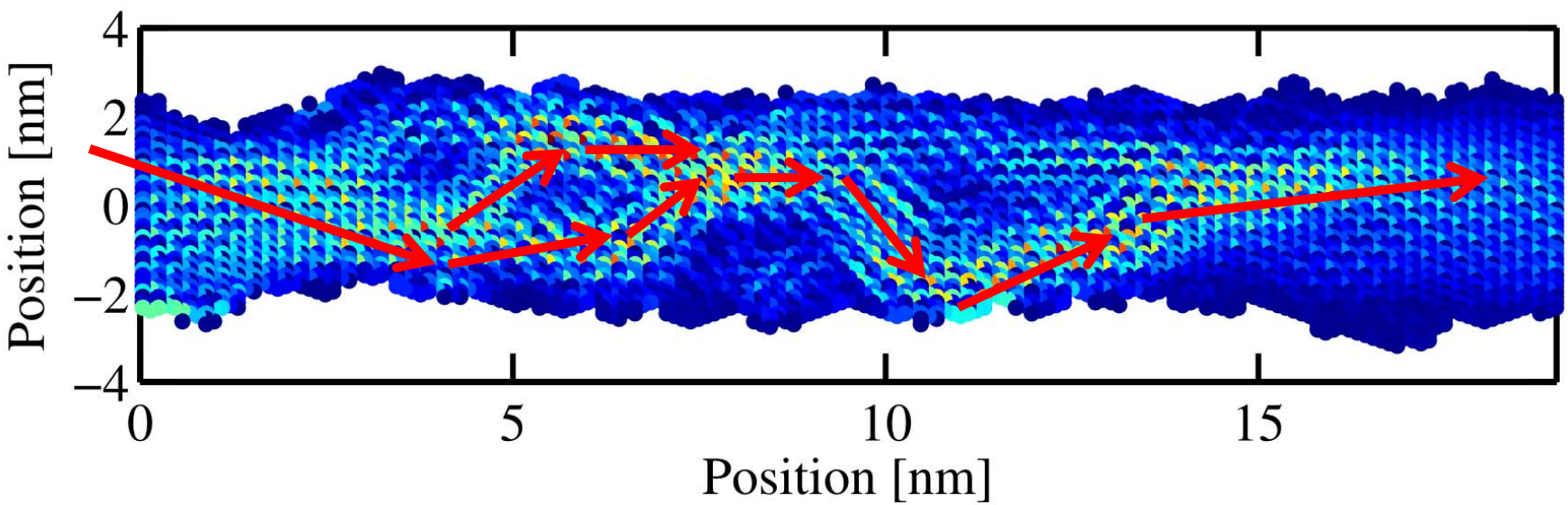
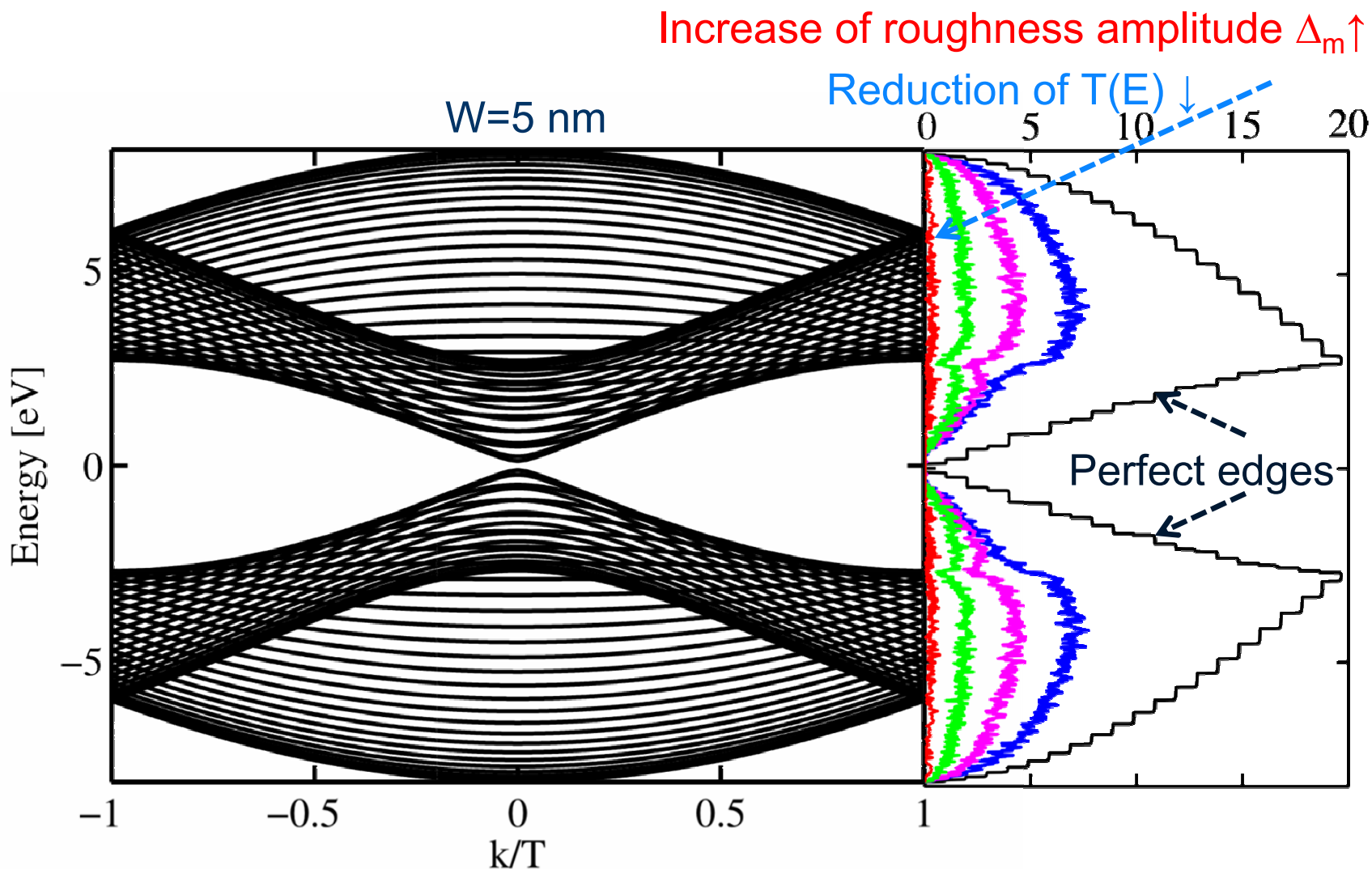


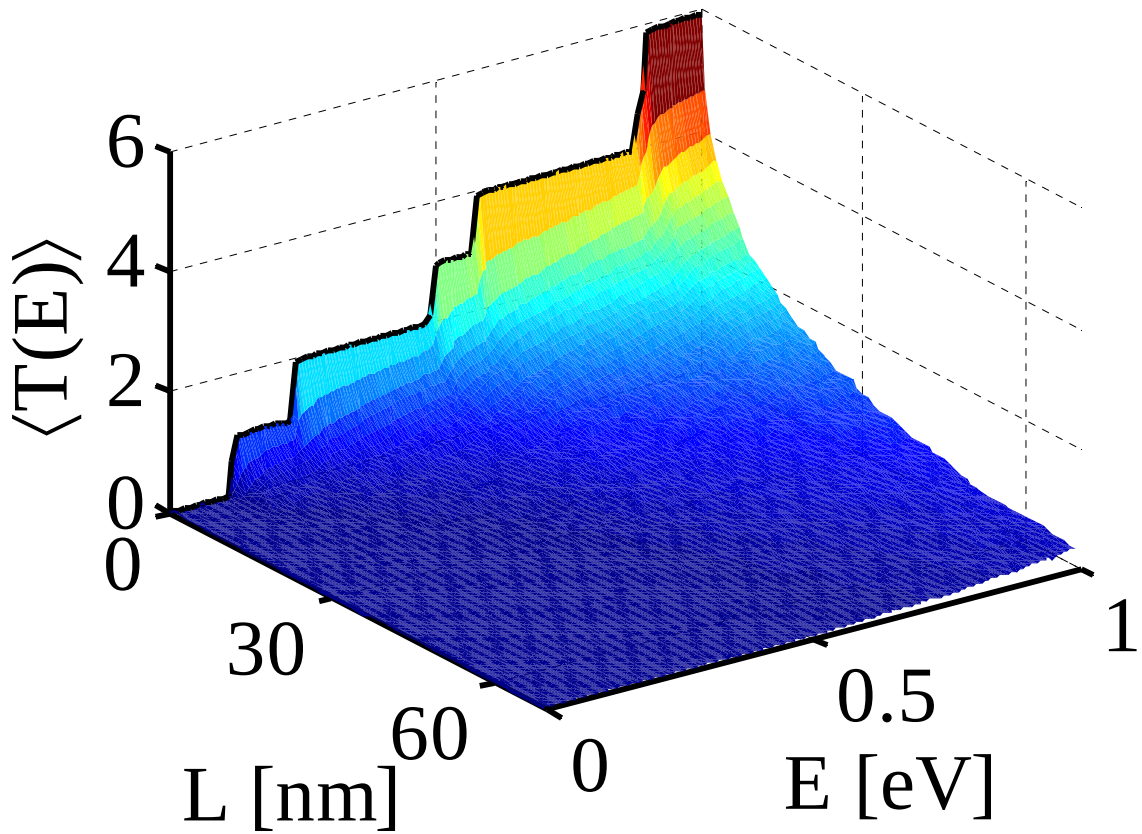
The Effect of Roughness Parameters

- **Transmission function**



The Role of Length

- **Transmission as a function of length and energy**



W = 5 nm

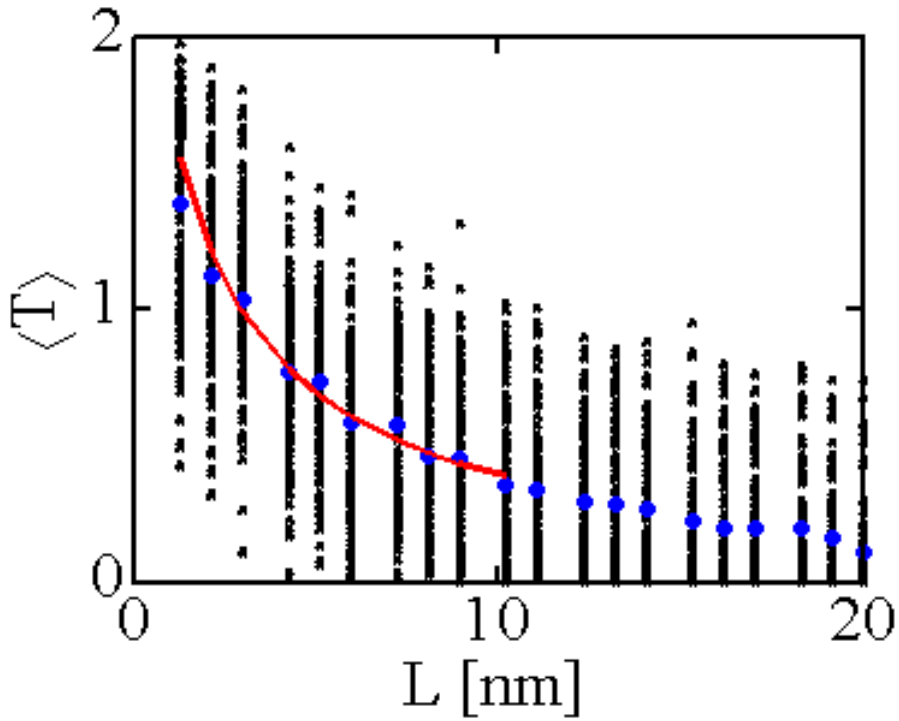
Δ_m = 0.5 nm

L_m = 3 nm

Diffusive Transport

- **Transmission as a function of length**

$$\langle T(E) \rangle = \frac{N_{\mathrm{ch}}(E)}{1 + L/\lambda}$$

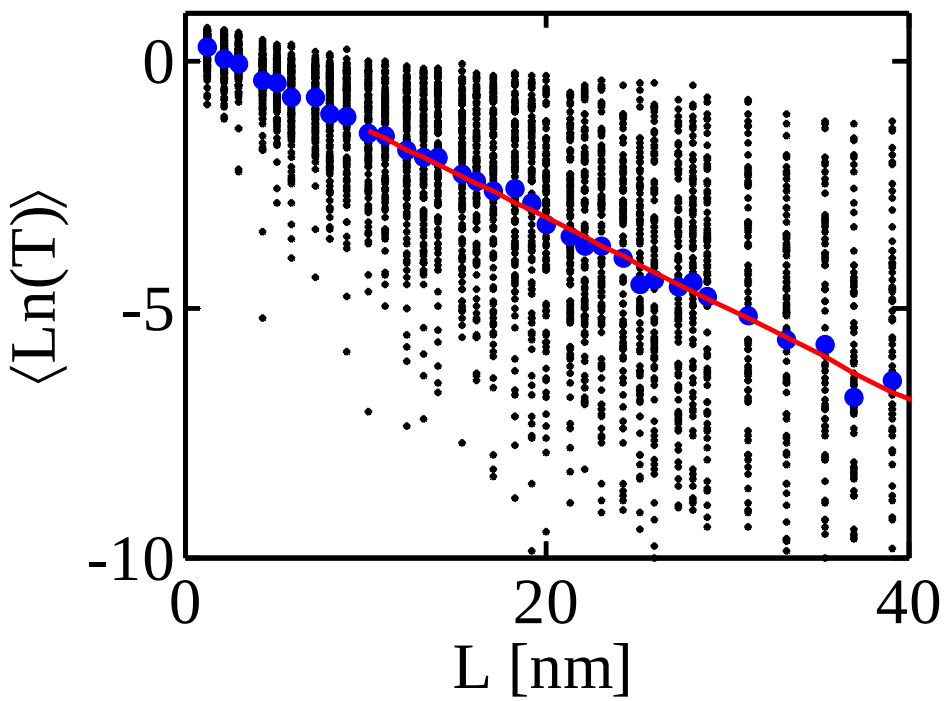


- E = 0.4 eV
- $N_{ch} = 2$
- $\lambda \approx 3$nm

Localization Regime

- **Transmission as a function of length**

$$\langle \ln \{T(E)\} \rangle \propto -L/\xi$$

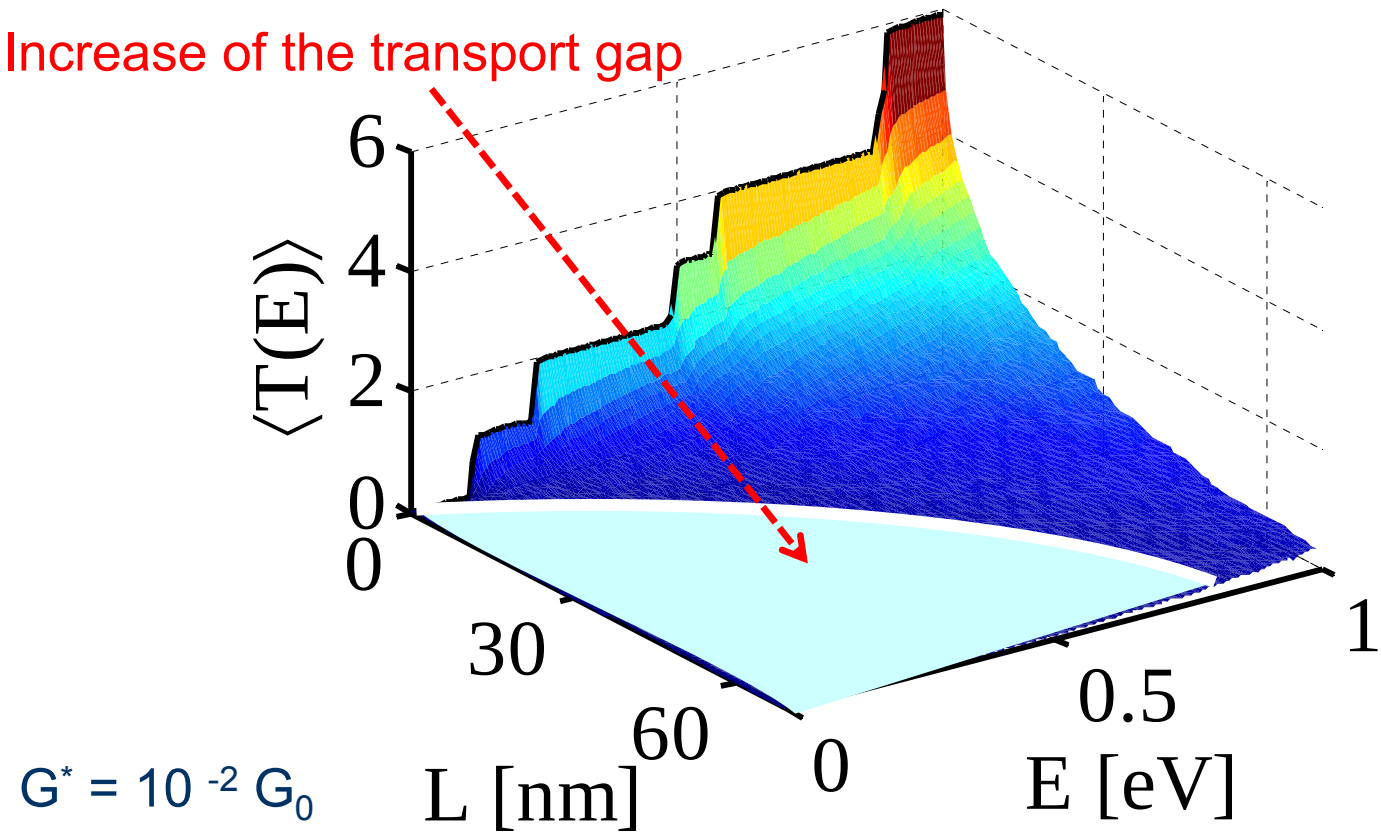


$\xi \approx 6$ nm

Localization Regime

- **Transport bandgap**

$$\xi/\lambda \propto N_{\mathrm{ch}}(E)$$



W = 5 nm

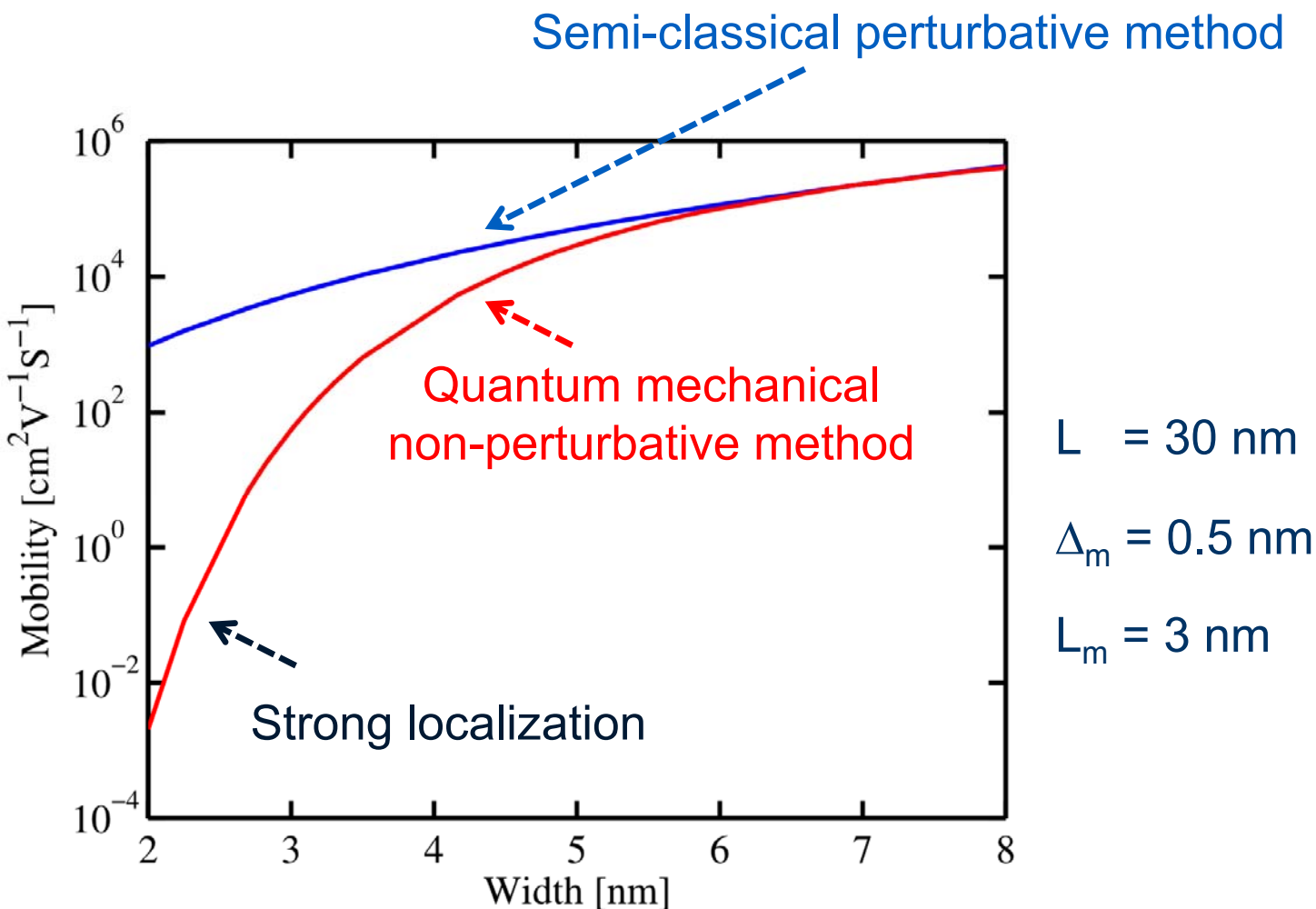
Δ_m = 0.5 nm

L_m = 3 nm

$G^* = 10^{-2}\ G_0$

Localization Regime

- **Mobility**



Conclusions

- The localization length is proportional to N_{ch} $\longrightarrow$ at low energies only few sub-bands contribute and the localization length is short, at higher energies the localization length increases. The effective transport energy gap increases for GNRs with rough edges.