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SPRING COLLEGE ON SCIENCE AT THE NANOSCALE
(24 May - 11 June 2004)

ELECTRONIC / THERMAL TRANSPORT - Part I

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These are preliminary lecture notes, intended only for distribution to participants.

Electric and Thermal Transport in Nanoscale Materials –Part I

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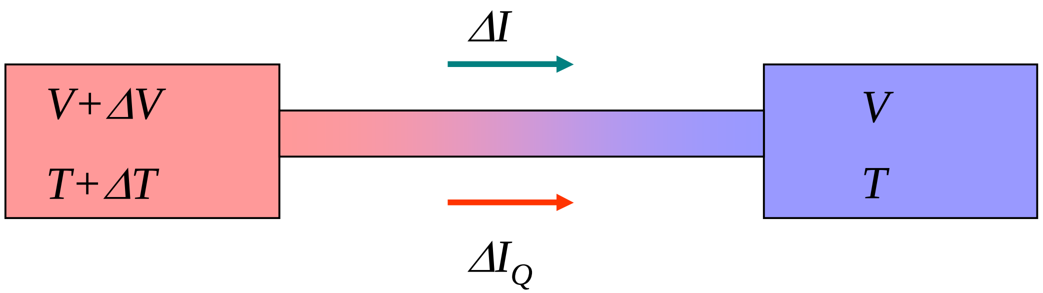
COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

Columbia University and the National Science Foundation
Center for Electron Transport in Molecular Nanostructures

Outline

- Charge Transport and Energy Dissipation
- Mesoscopic Heat Transport Measurements
- Mesoscopic Thermoelectric Effects (Wed)
- Field Effect Transport in 2D Crystallites (Thr)

Charge, Energy and Entropy Transport



Linear Response Regime

$$\Delta V = R\,\Delta I - S\,\Delta T$$

$$\Delta I_Q = \Pi\,\Delta I - K_{th}\,\Delta T$$

R : electric resistance (electron)

K_{th} : thermal conductance (electron&phonon)

S : Thermopower (electron+phonon)

Π: Peltier Coefficient

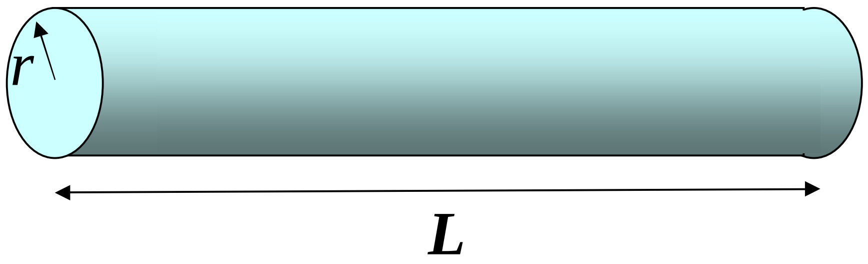
Onsager relation

$$\Pi = S\,T$$

Wiedemann-Franz Law:

$$\frac{K_{th}}{1/R} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T$$

Classical Channel



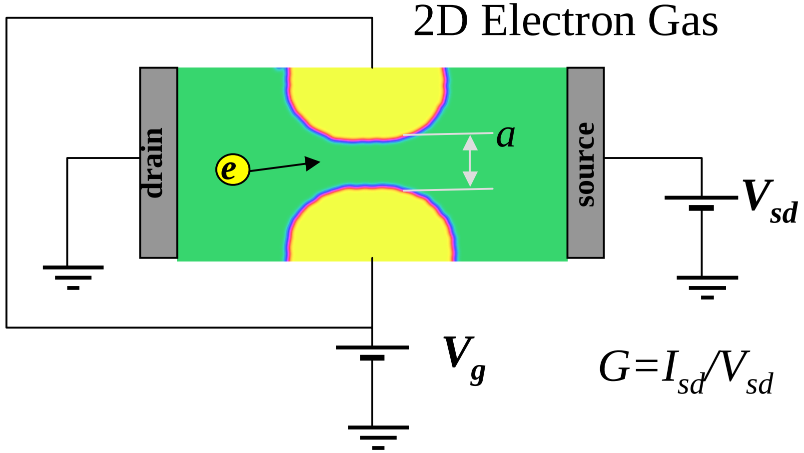
Electric Conductance

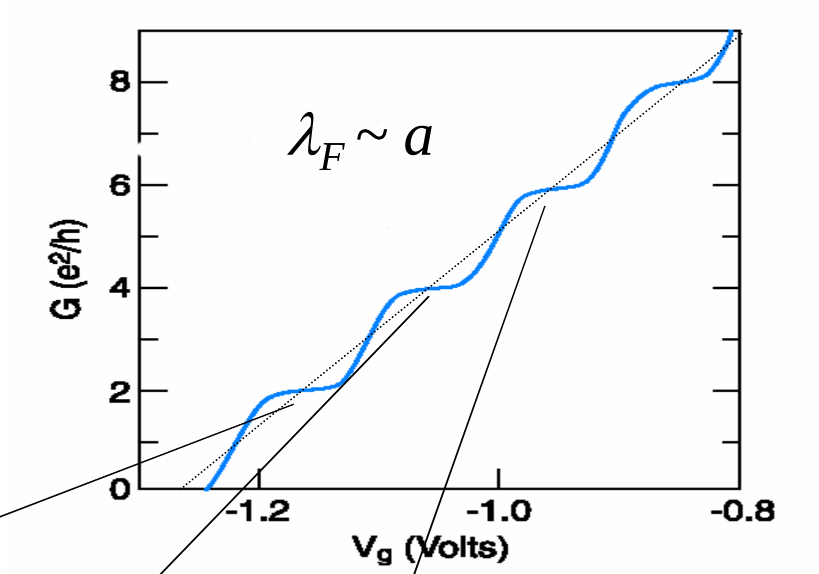
$$G = 1/R = \sigma \pi r^2/L$$

Thermal Conductance

$$K_{th} = \kappa \pi r^2/L$$

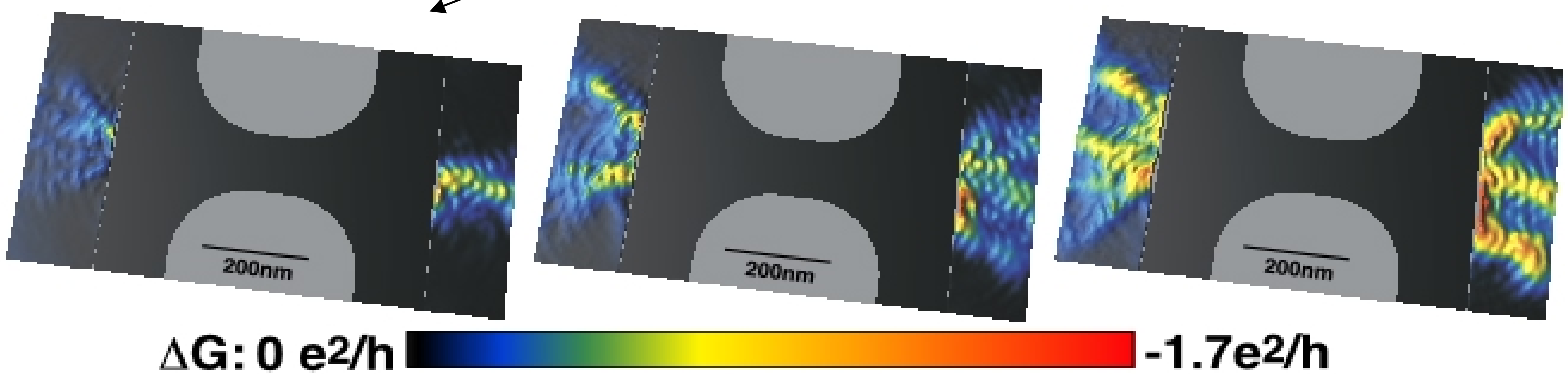
Conductance Quantization in Quantum Point Contact





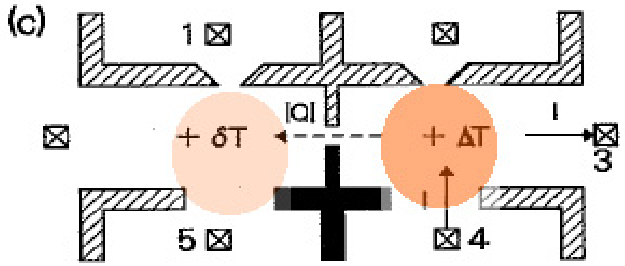
Quantum Conductance: $g_0=e^2/h$

M. Topinka *et al*, *Science* (2000)

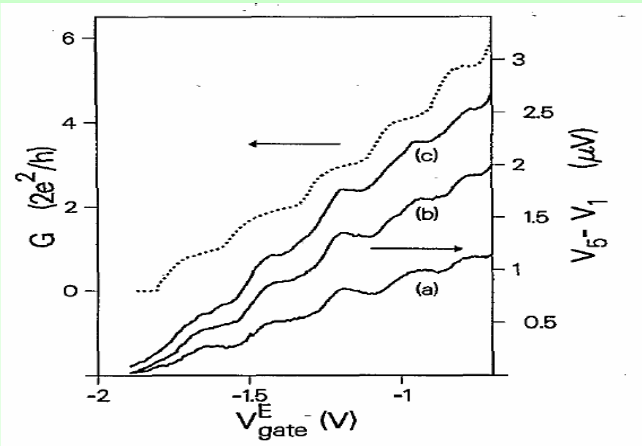


Quantization of Thermal Properties in Mesoscopic Electron Systems

Quantum point contact



Electronic thermal conductance quantization
(Molenkamp *et al*. PRL, 1991)



Quantum Thermal Conductance

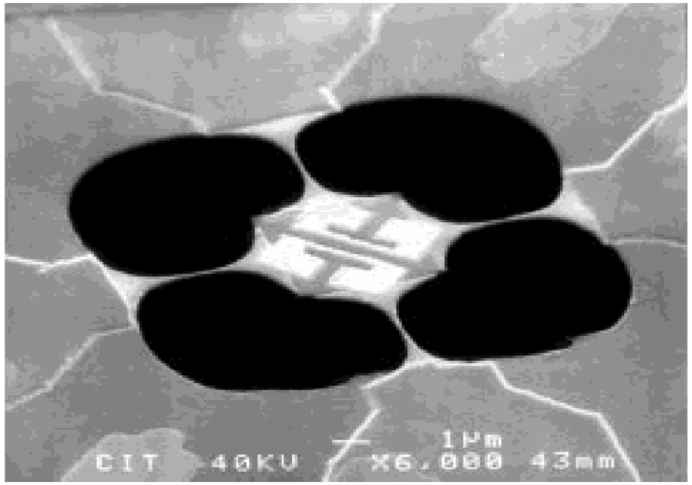
$$g_0^{th} = \pi^2 k_B^2 T/(3h)$$

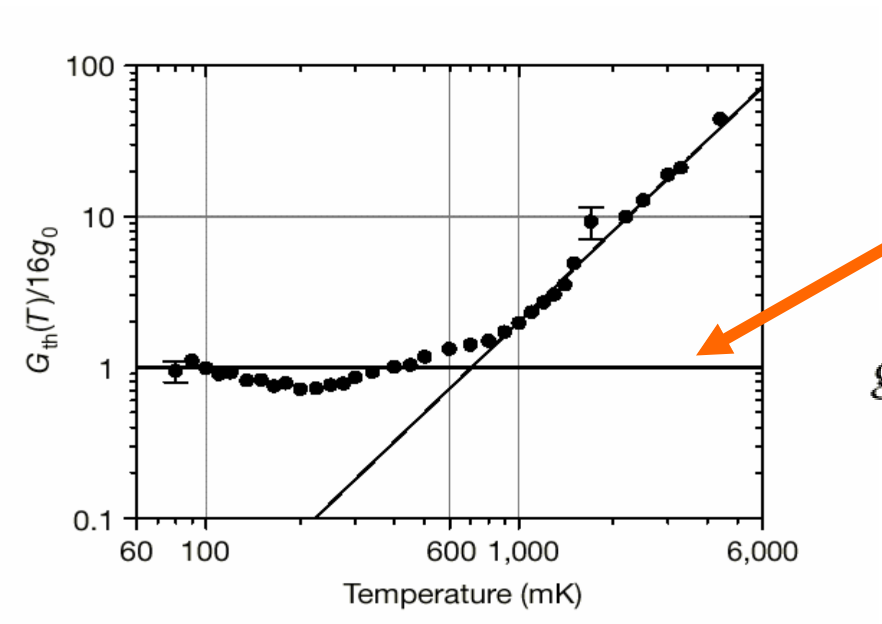
Wiedemann-Franz Law:

$$\frac{g_0^{th}}{g_0^{el}} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T$$

Thermal Conductivity Quantization in Phonon System

Phonon thermal conductance quantization
in Silicon Nitride Membrane Nanostrucure
(Schwab *et al.*, Nature, 1999)



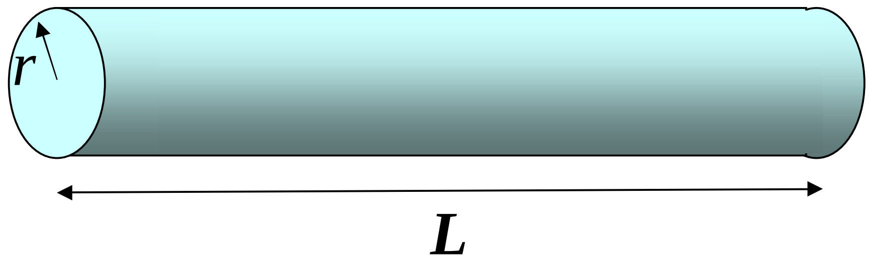


Quantum thermal conductance

$$g_0^{th} = \pi^2 k_B^2 T/(3h)$$

universal thermal quanta

Quantum Transport Channel



$r \sim \lambda_F, \lambda_{th}$

# of channel

Electric Conductance

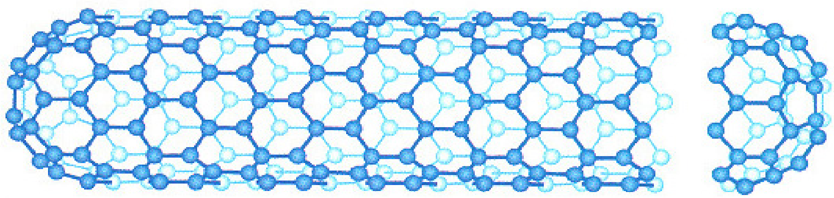
$G = \sigma \pi r^2/L$ ⟶ $G = N_{ch}^{e} g_0^{e}$; $g_0^e = e^2/h$

Thermal Conductance

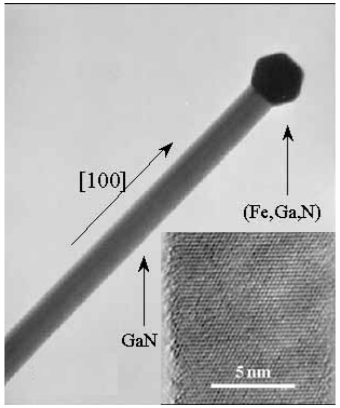
$K_{th} = \kappa \pi r^2/L$ ⟶ $K_{th} = N_{ch}^{th} g_0^{th}$; $g_0^{th} = \pi^2 k_B^2 T/(3h)$

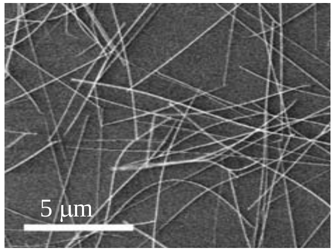
Synthesized 1 Dimensional Nanoscale Materials

Carbon Nanotubes



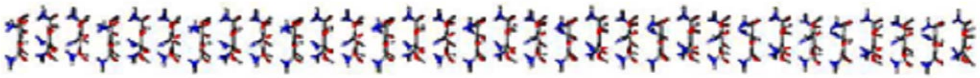
Semiconductor Nanowires



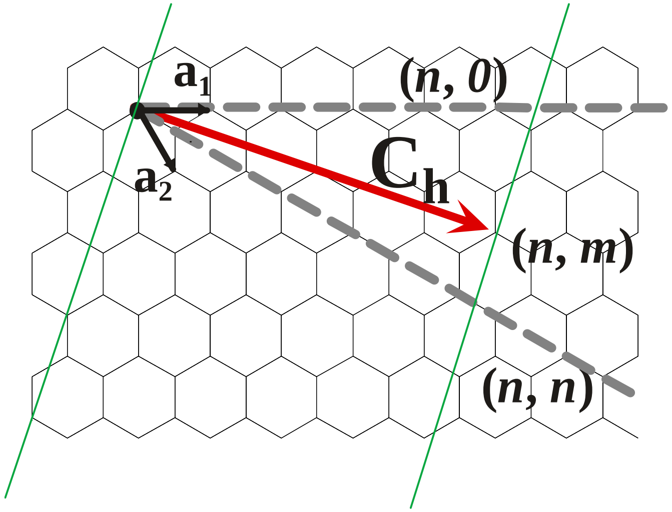


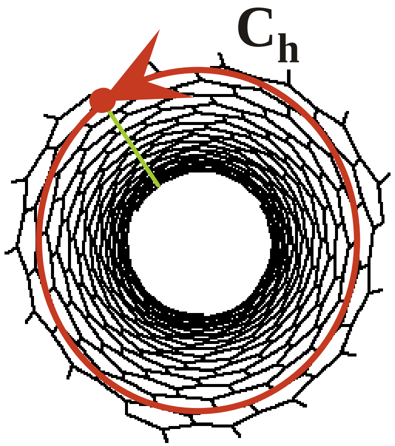
(Lieber et al.)

Organic Nanowires



Carbon Nanotube: Electronic Structure

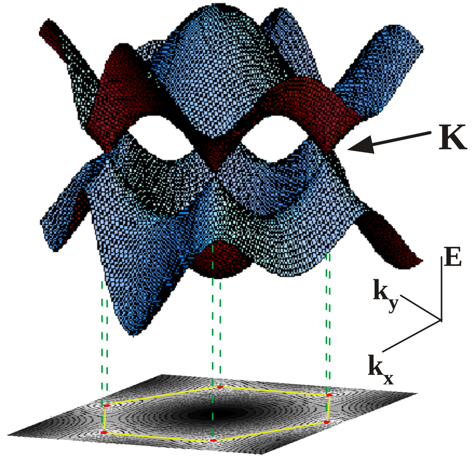




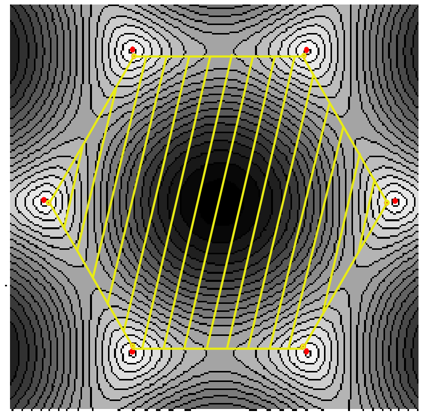
Rolling up graphene along C_h imposes a Periodic boundary condition :

$$C_h \cdot \mathbf{k} = 2\pi\, q$$

π/π^* band of Graphene

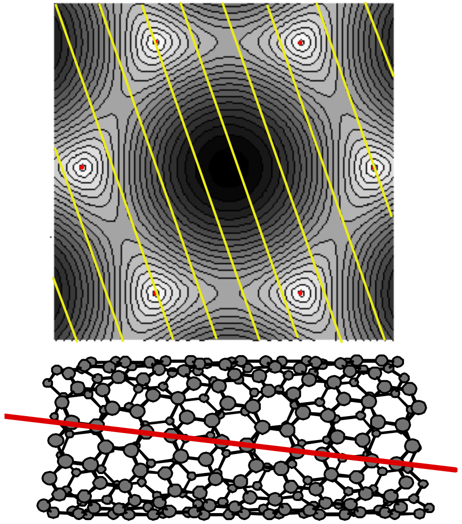


set of allowed states



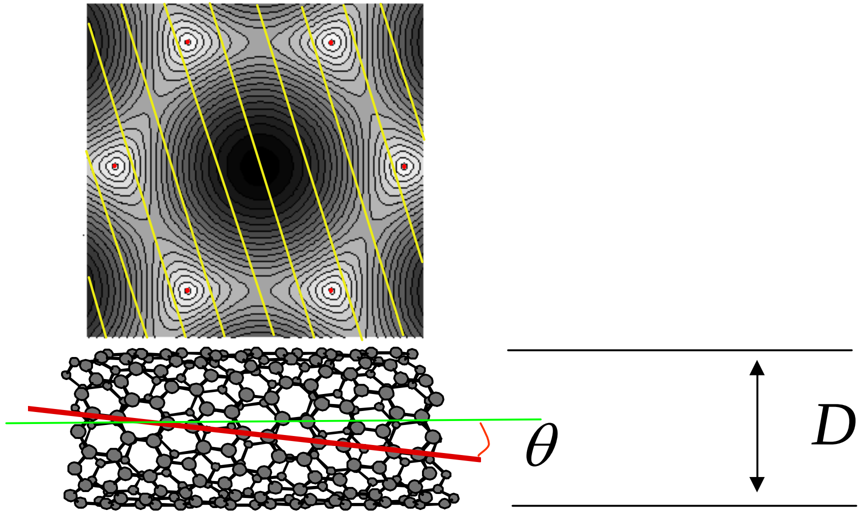
Metallic and Semiconducting Nanotubes

Metallic Nanotube



n - m = 3q

Semiconducting Nanotube



n - m ≠ 3q

$$D = |\mathbf{C}_h|/\pi = \sqrt{3}a_{cc}(m^2 + mn + n^2)^{1/2}/\pi$$

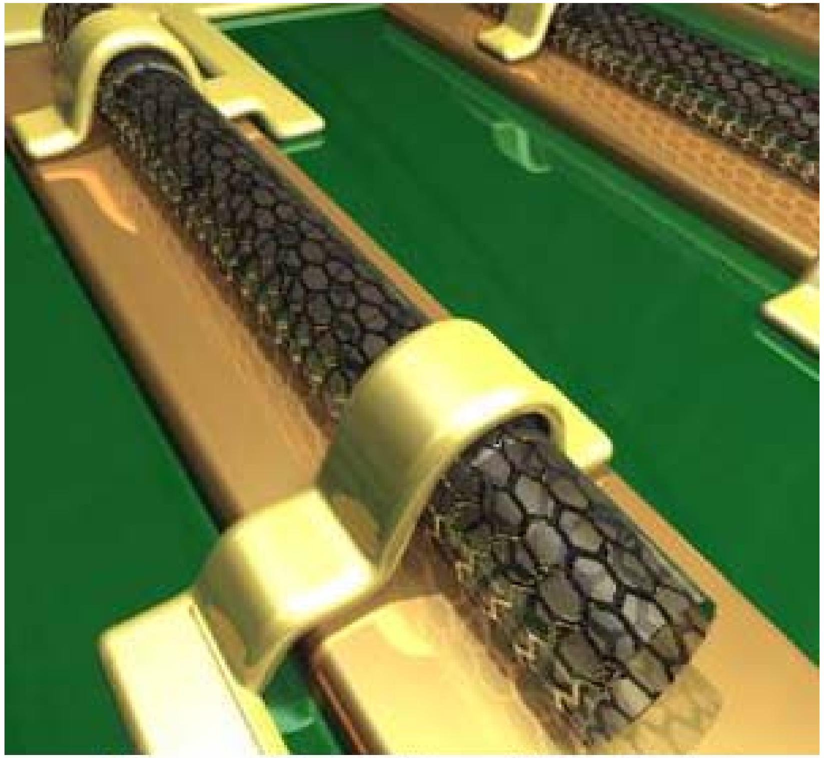
$$\theta = \tan^{-1}\left[(\mathbf{C}_h \times \mathbf{a}_1)\cdot\hat{\mathbf{z}}/\mathbf{C}_h\cdot\mathbf{a}_1\right] = \tan^{-1}\left[\sqrt{3}m/(m+2n)\right].$$

Electrical Transport in Carbon Nanotube

Metallic or semiconducting:
depending on chirality&diameter

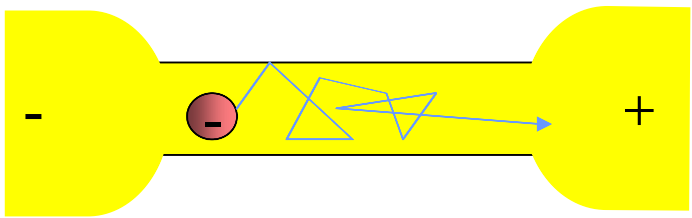
Exotic 1D electron system: Luttinger liquid?

Ballistic electron transport in metallic tube:
even at room temperature

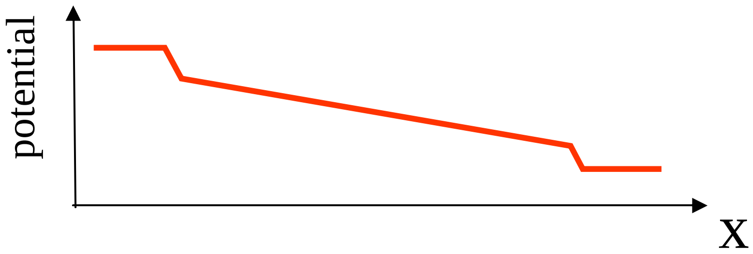


Artist's conception of a gated nanotube transistor logic circuit. Bachtold et al., *Science* **294** (2001) 1317.

Ballistic Electron Transport

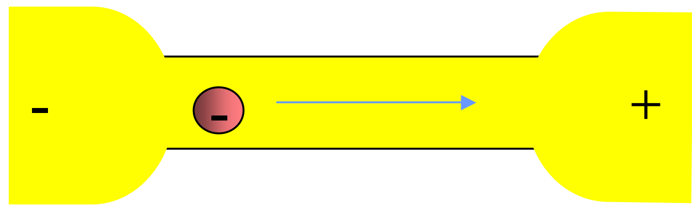


Diffusive

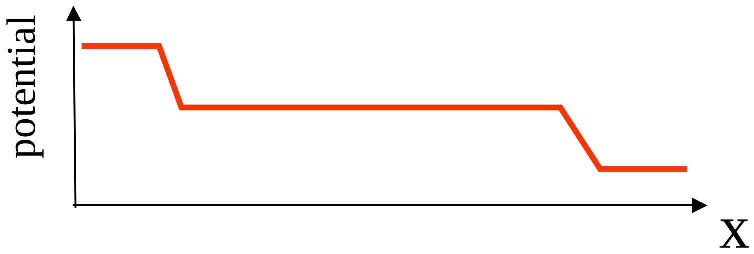


Ohmic Conductor

$$R = \rho L/A$$



Ballistic

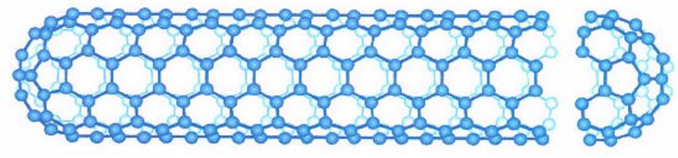


Quantum Transport

$$R = h/2e^2N$$

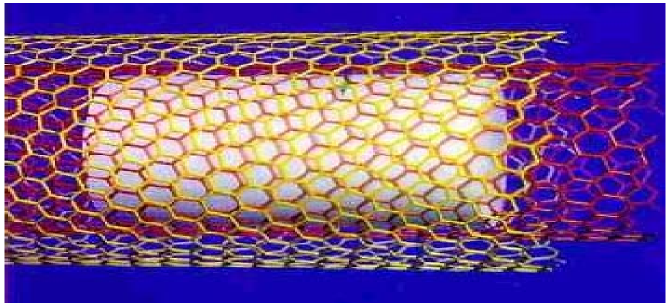
Charge Transport in Nanotubes

Metallic Singlewall Nanotube :



Ballistic at low bias: (Schönenberger *et al.*, 1999, Bachtold *et al.*, 2000, Z. Yao *et al.*, 2000, Liang *et al.*, 2001)

Multiwall Nanotube :

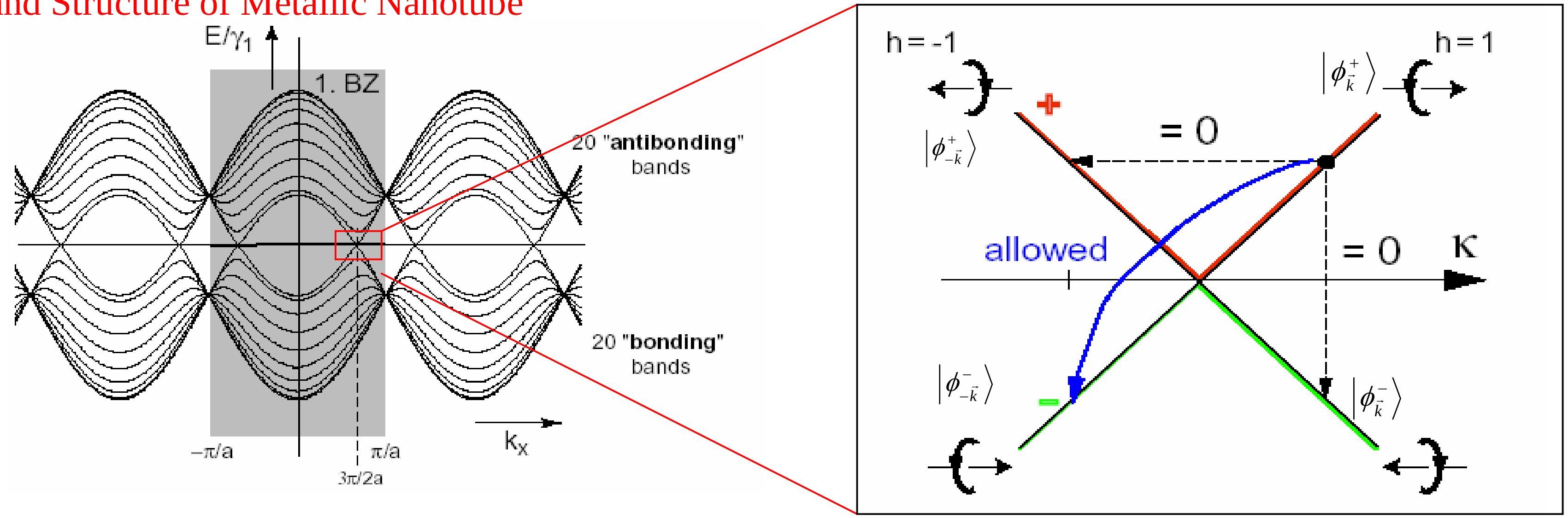


Ballistic (S. Frank *et al.*, 1998)

Diffusive (C. Schönenberger *et al.*, 1999, Bachtold *et al.*, 2000)

Ballistic Electron Transport in Carbon Nanotube

Band Structure of Metallic Nanotube



$$H_{eff} \approx \hbar v_f \vec{\sigma} \cdot \vec{k}_{2D}$$

$\vec{\sigma}$: Pauli matrices

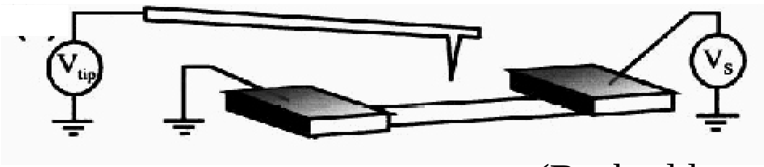
$$|\langle \phi^+_{\vec{k}} | \langle \phi^+_{\vec{k}} \rangle|^2 = 1$$
$$|\langle \phi^-_{\vec{k}} | \langle \phi^-_{\vec{k}} \rangle|^2 = 1$$
$$|\langle \phi^+_{\vec{k}} | \langle \phi^-_{-\vec{\kappa}} \rangle|^2 = 1$$
$$\langle \phi^+_{\vec{k}} | \langle \phi^+_{-\vec{\kappa}} \rangle = 0$$
$$\langle \phi^-_{\vec{k}} | \langle \phi^-_{-\vec{\kappa}} \rangle = 0$$

Suppression of long wavelength BACK scattering

Ando et al., 1998

Measurement of Electrical Field Distribution

Electric Force Microscope (EFM)

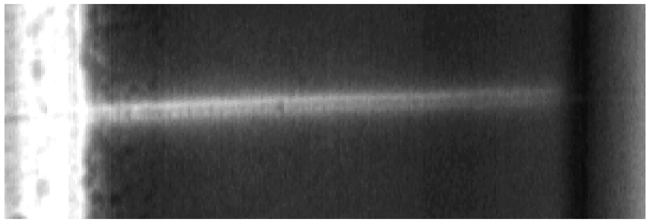


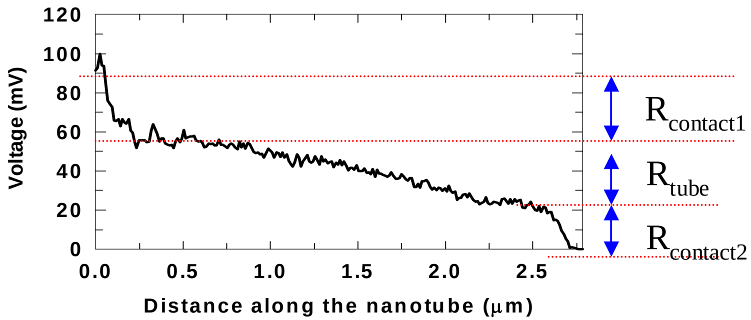
(Bachtold *et al.*, 2000)

AC EFM : probing local electric field

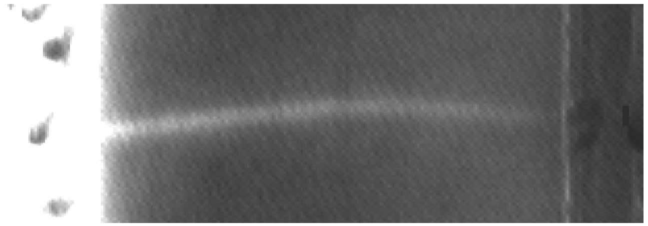
$$F_{ac}(w) = (dC/dz)(V_{tip} + \phi)V_s(w)$$

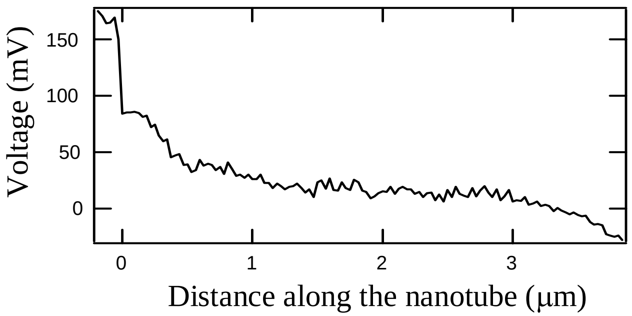
Multiwall Nanotube: diffusive



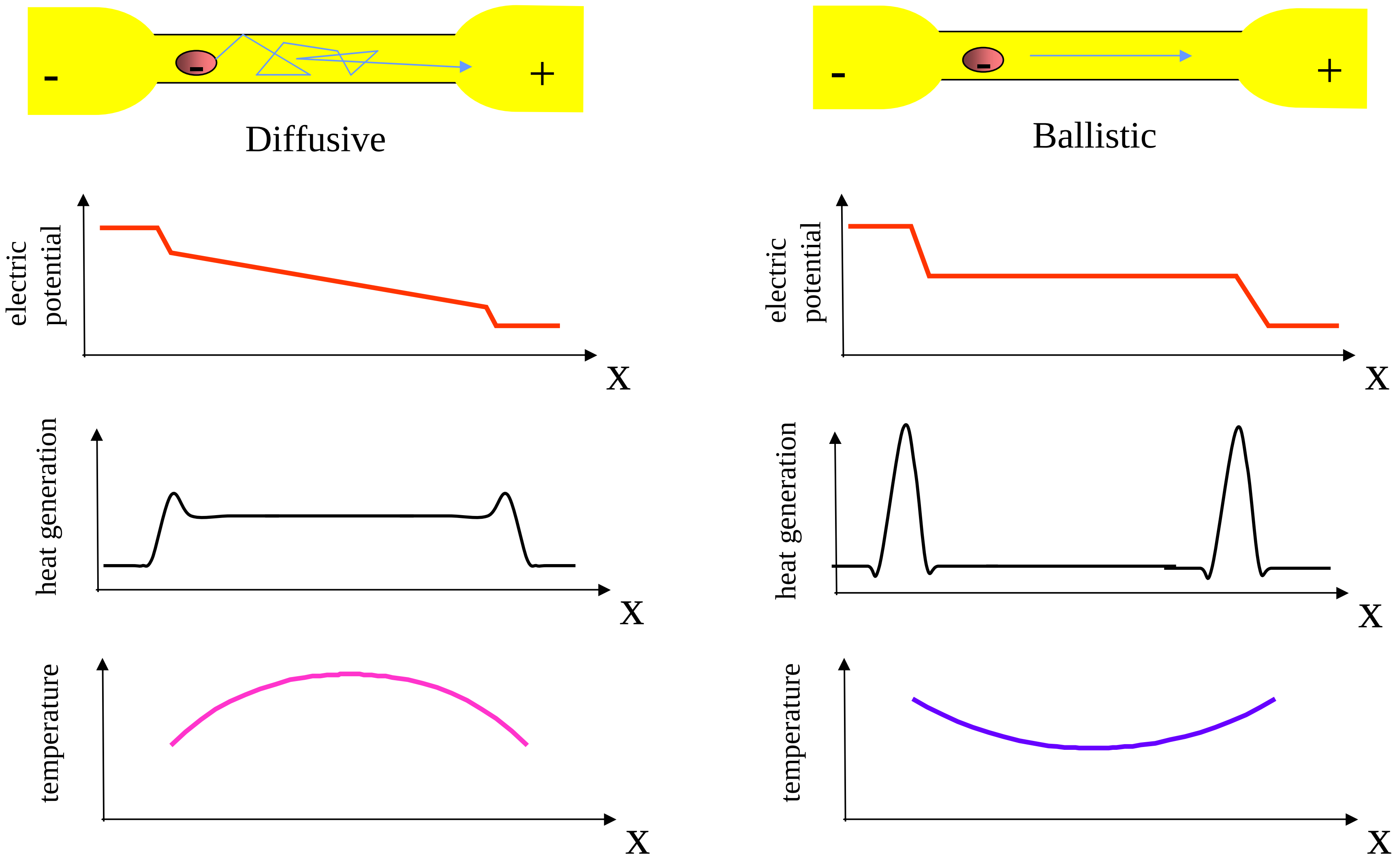


Singlewall Nanotube: ballistic

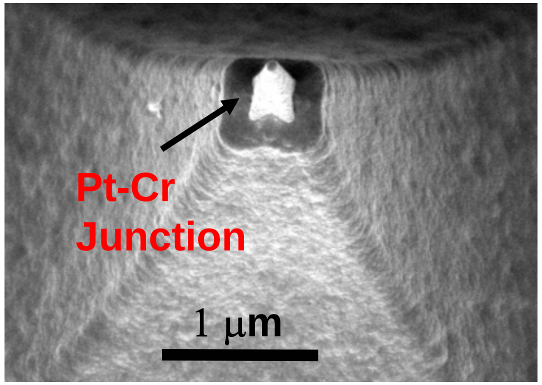


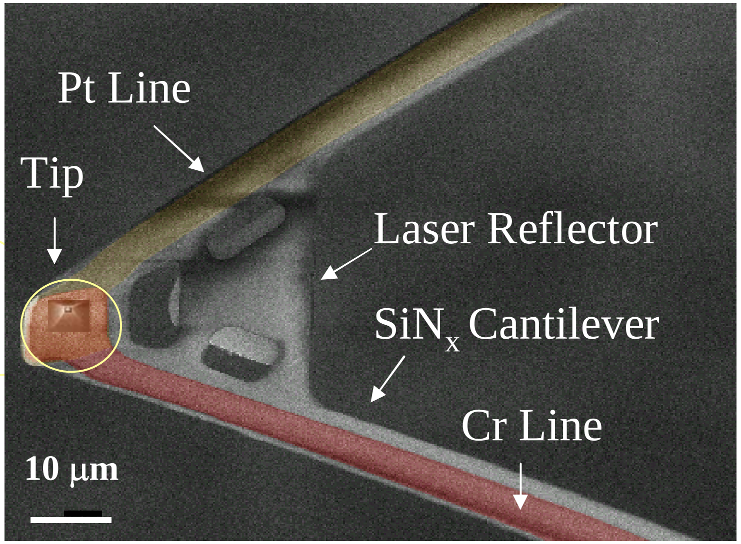


Ballistic Electron Transport

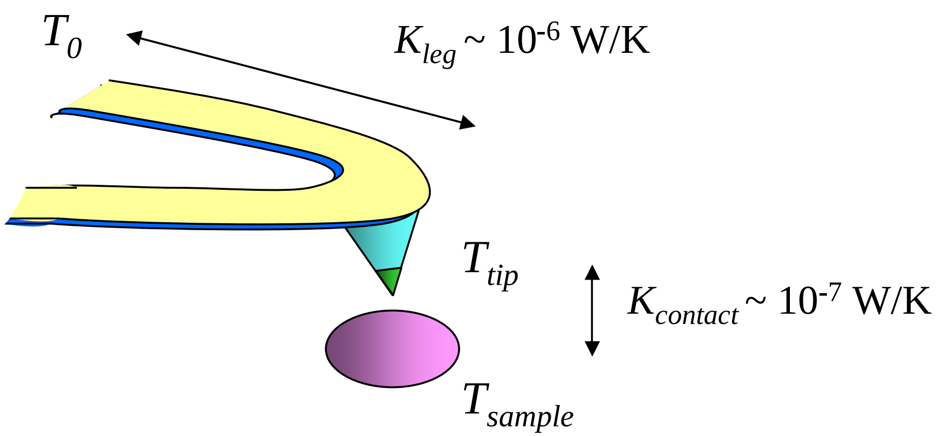


Local Temperature Probe





Probing local phonon temperature



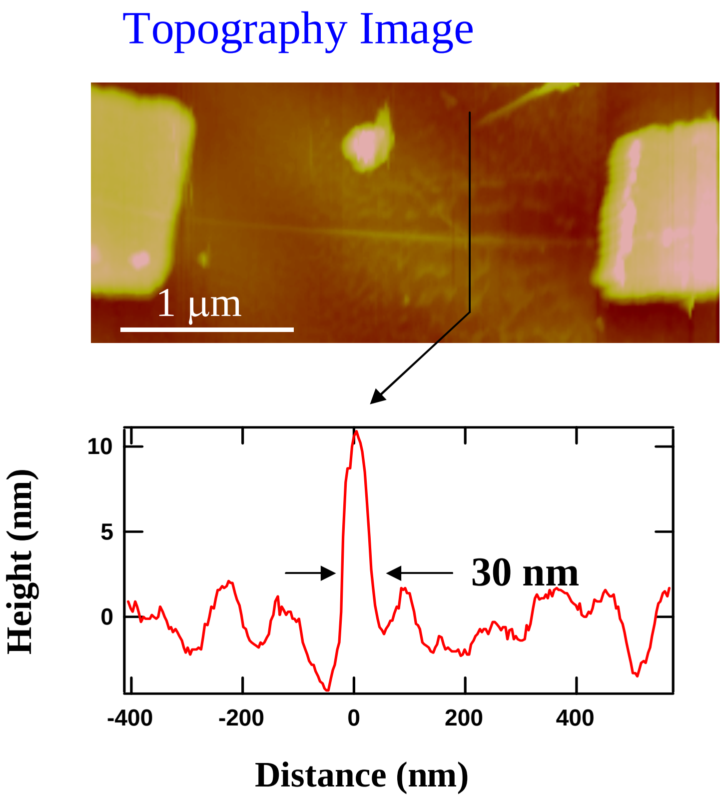
Temperature reading :

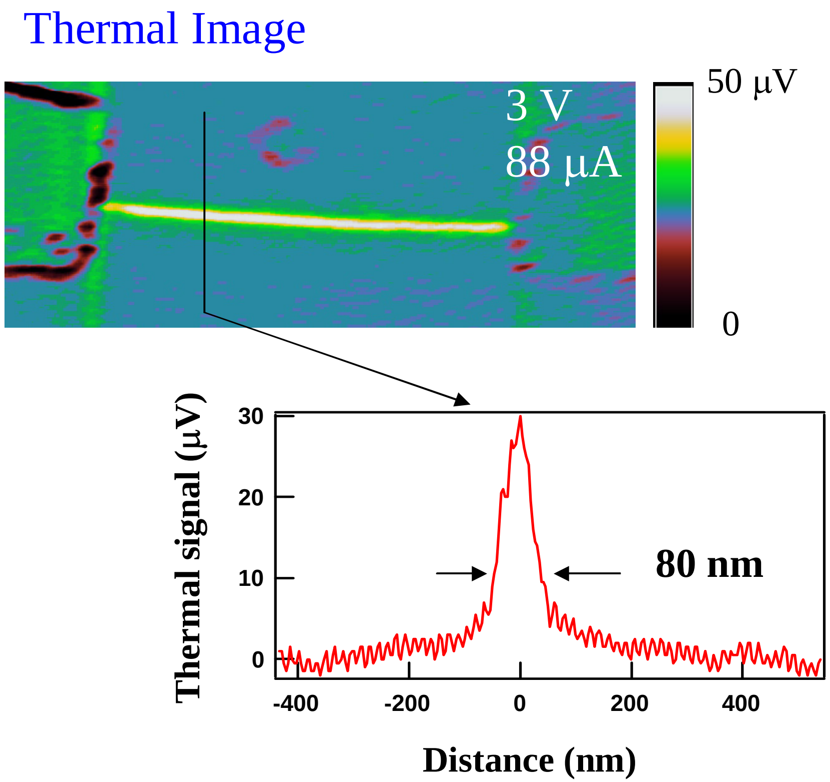
$$\Delta T_{saample} = \frac{K_{leg}}{K_{contact}} \Delta T_{tip}$$

t

Scanning Thermal Probe on Nanotube: Calibration

Multiwall Nanotube on 100 nm SiO/Si Substrate





Seebeck coefficient of probe : 13.5 µV/K

Temperature Distribution of Diffusive Conductor

1d Diffusion Equation:

$$K\frac{d^2T}{dx^2} = -P(x) + a\left(T(x) - T_s(x)\right)$$

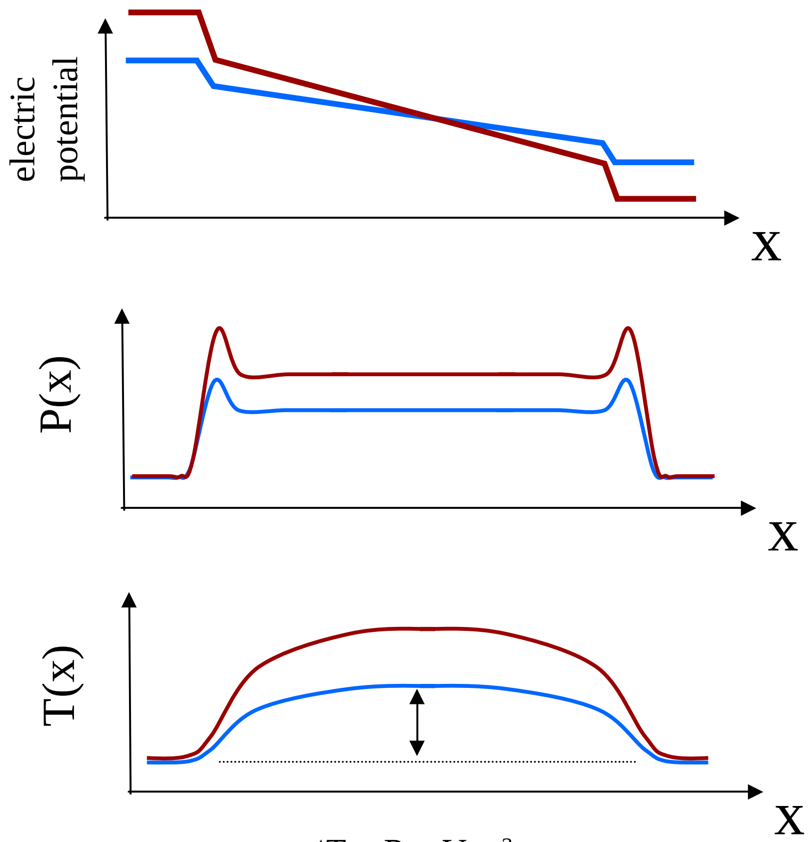
Thermal conductance

Local power dissipation

Coefficient of Substrate coupling

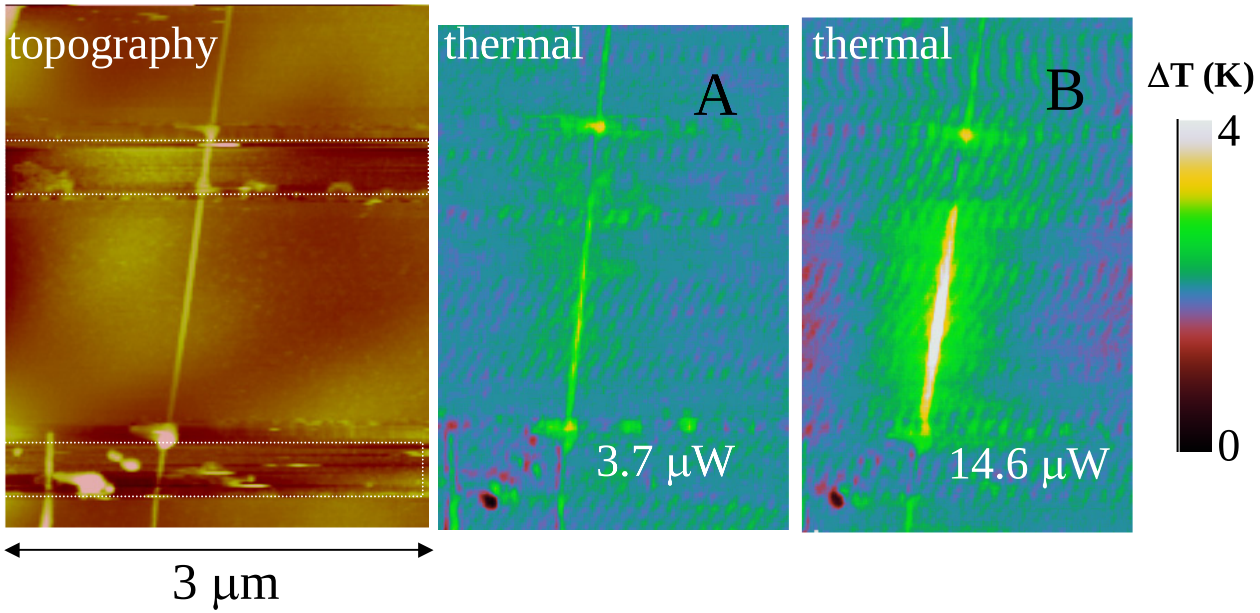
Substrate temperature

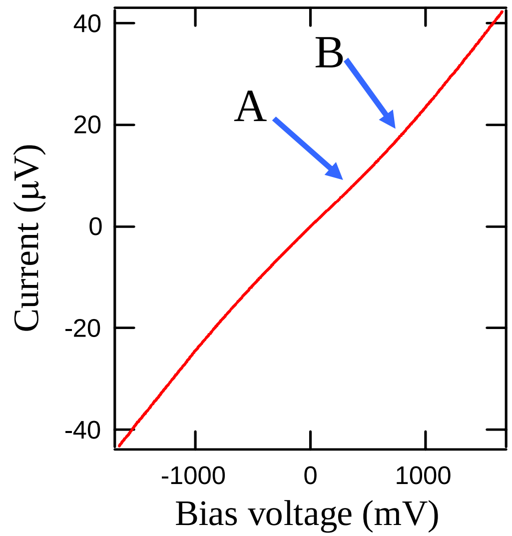
Dissipative Transport

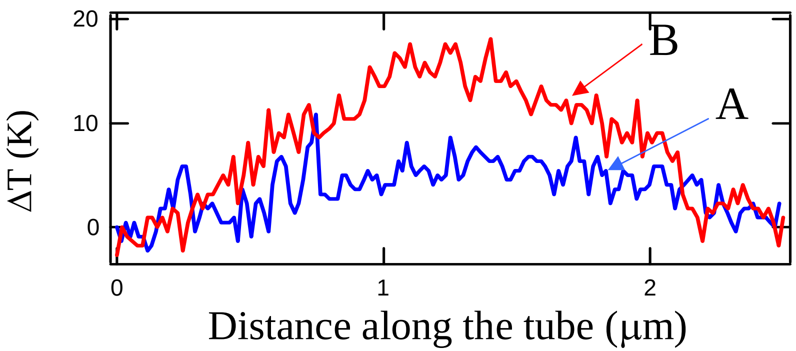


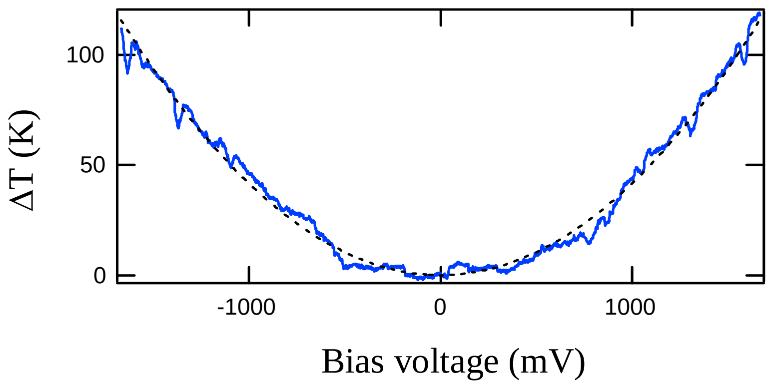
$\Delta T \sim P \sim V_{bias}^{2}$

Bulk Dissipation in Multiwall Nanotube



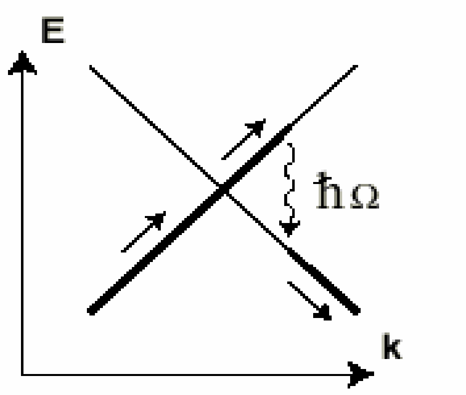






Single Walled Nanotube: Energy Dissipation at High Field

- Optical Phonon Emission: from ballistic to diffusive

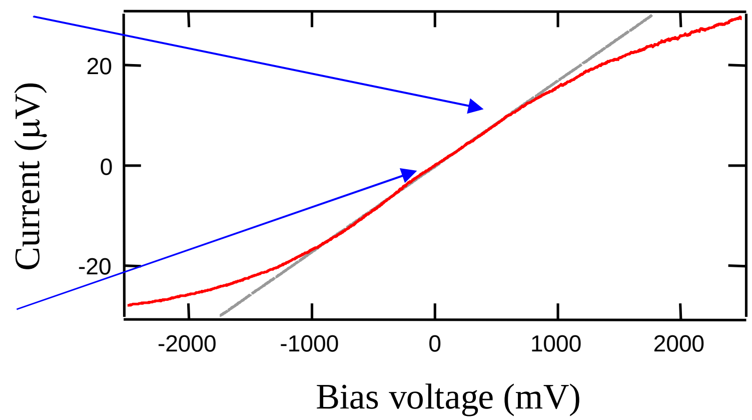


Onset of optical phonon ~ 150 meV

Onset of optical phonon scattering

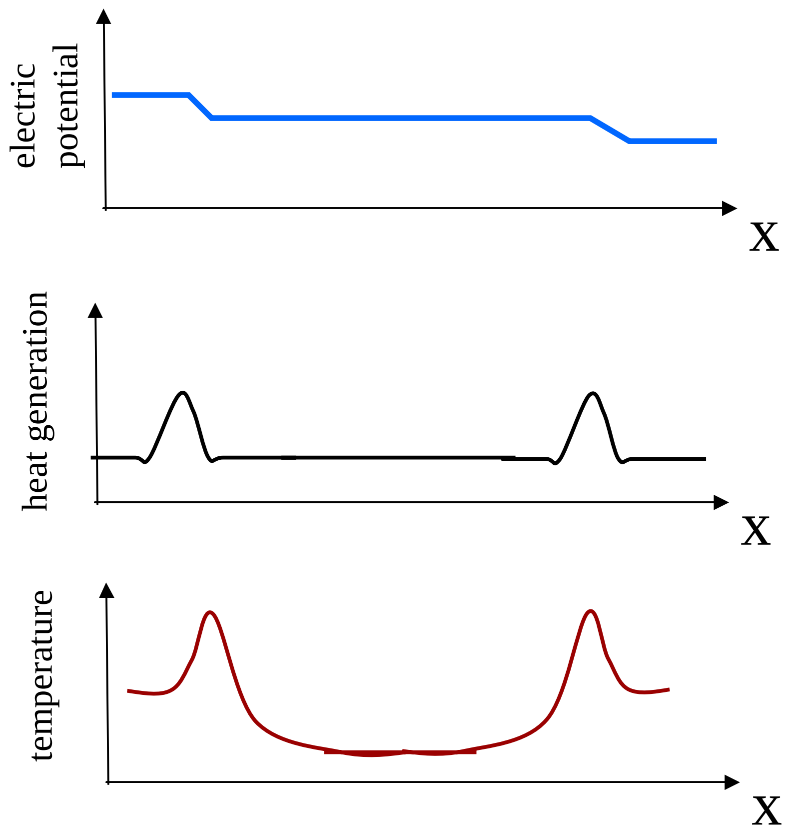
(Z. Yao *et al*., 2000)

linear response regime, ballistic.

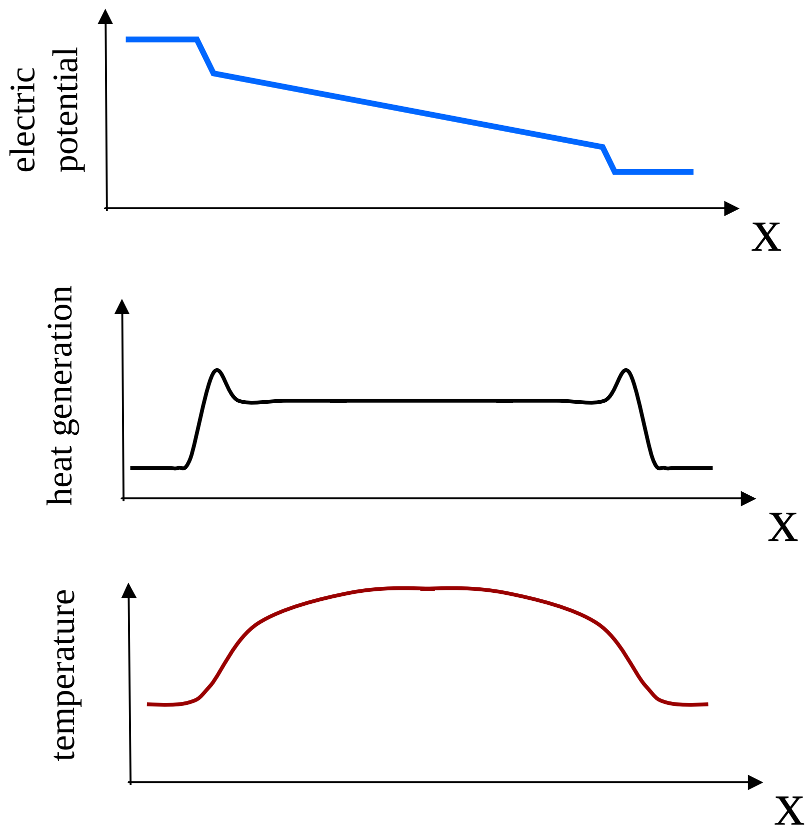


Low Bias and High Bias Transport in SWNT

Low bias: ballistic



High bias: dissipative



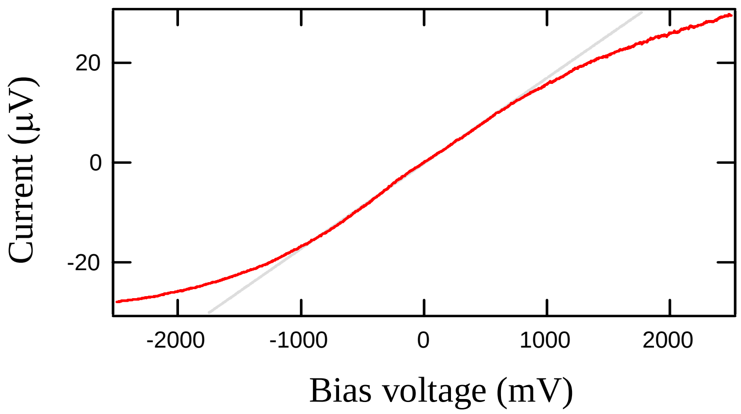
Ballistic to Diffusive Transport

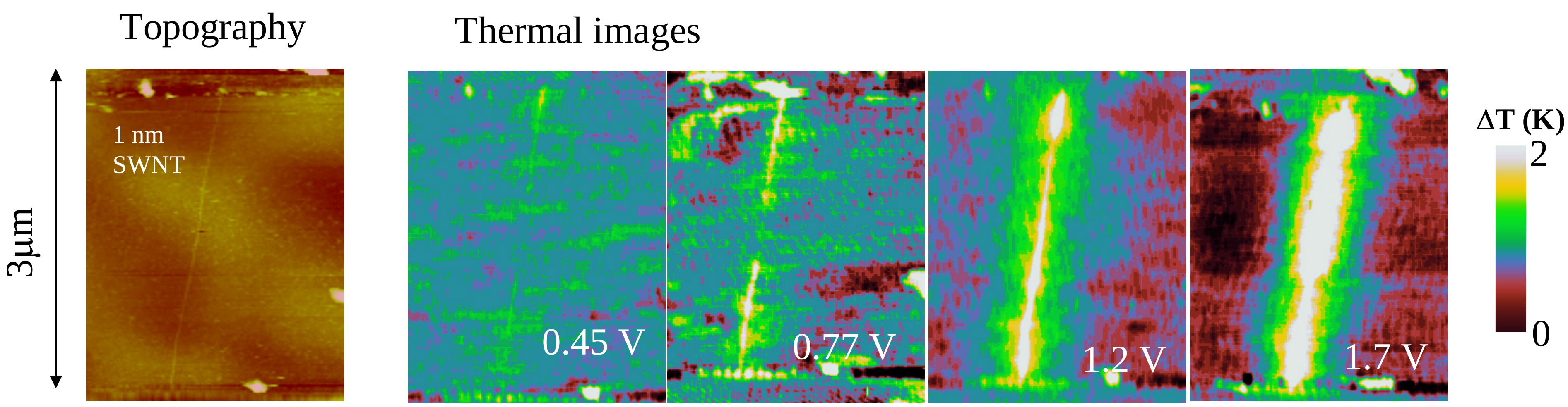
Low bias: ballistic

→ junction dissipation

High bias: diffusive

→ bulk dissipation





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Measurement of Energy Flow

Thermal Conductivity

$$K_{th} = \frac{dQ}{dT}$$

Phonon Thermal Conductivity of Materials

Kinetic Theory

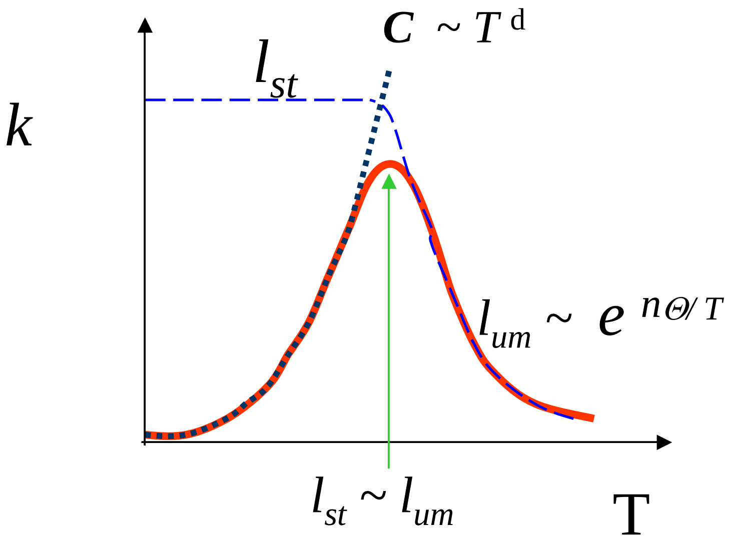
$$k = \frac{1}{3} C\, v_s\, l$$

thermal conductivity — specific heat — sound velocity — phonon mean free path

Specific heat :

If $T << \Theta$, $\quad C \sim T^{d}$ (d:dimension)

If $T > \Theta$, $\quad C \sim constant$



Mean free path:

$$\frac{1}{l} = \frac{1}{l_{st}} + \frac{1}{l_{um}}$$

Static scattering: $\quad l_{st} \sim constant$

Umklapp scattering: $\quad l_{um} \sim e^{+n\Theta/T}$