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Electric Transport in Carbon Nanotubes and Graphene at High Field

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Transport, current saturation and hot phonons at high bias in metallic nanotubes and graphene

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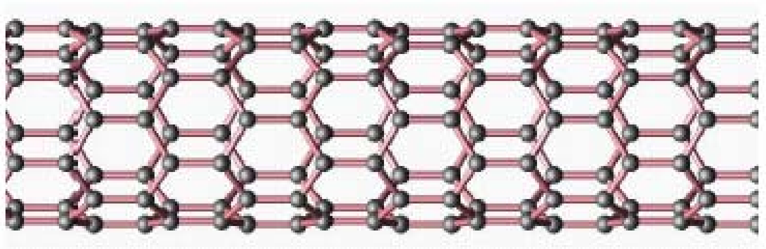
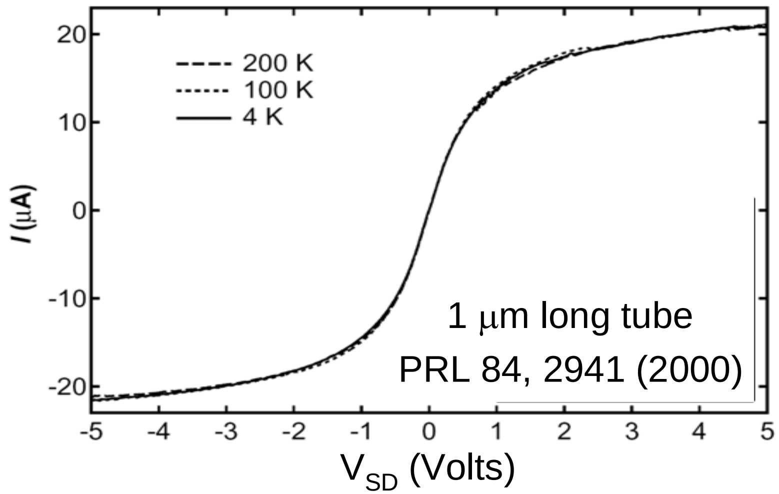
Motivations





Metallic Carbon nanotubes:

-Highest current density (~10^9 A/cm^2)

-Interconnects for tomorrow electronics but saturation of the current at high bias:

- What is the origin of the saturation?
- Can we improve the nanotube performances?
- Graphene at high bias: maximum current density? Graphene interconnects?

OUTLINE

- metallic carbon nanotubes:
  - -transport measurements at high bias
  - -scattering processes (DFT vs. experiments)
  - -Boltzmann for phonons and electrons, hot phonons
  - -cooling hot-phonons to improve performances
- graphene:
  - -transport measurements
  - -Boltzmann for phonons and electrons
  - -analysis of scattering lengths

OUTLINE

PART 1: Transport at high field in <u>metallic nanotubes</u>

-transport measurements at high bias

-scattering processes (DFT vs. experiments)

-Boltzmann for phonons and electrons, hot phonons

-cooling hot-phonons to improve performances

PART 2: Transport at high field in <u>doped</u> graphene

-experimental results on high-mobility graphene devices

-Boltzmann modeling of high field transport in graphene

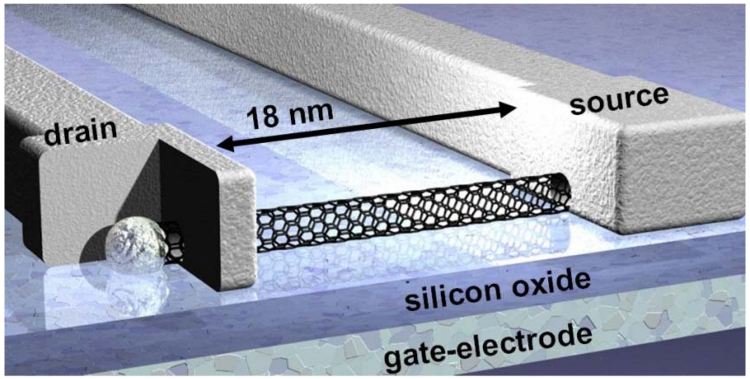
PART 3: Transport in graphene at high field near the <u>charge neutrality point</u>

-Boltmann (semiclassical) vs. quantum (tunneling) transport

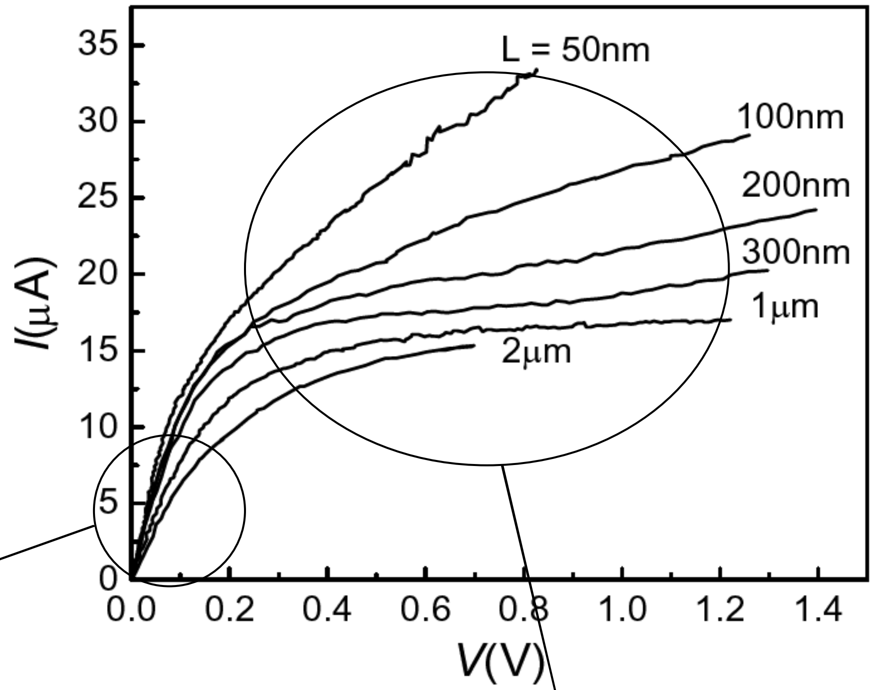
-Zener current in ballistic and disordered graphene: theory and experiment

metallic tubes on substrate

Park et al., Nano Lett. 4, 517 (04)



Experimental I/V of a nanotube transistor



V<0.2 V, ballistic regime

- resistance weakly depends on length in short tubes
- electron scattering length:

300 nm – 1600 nm

due to defects and acoustic phonons

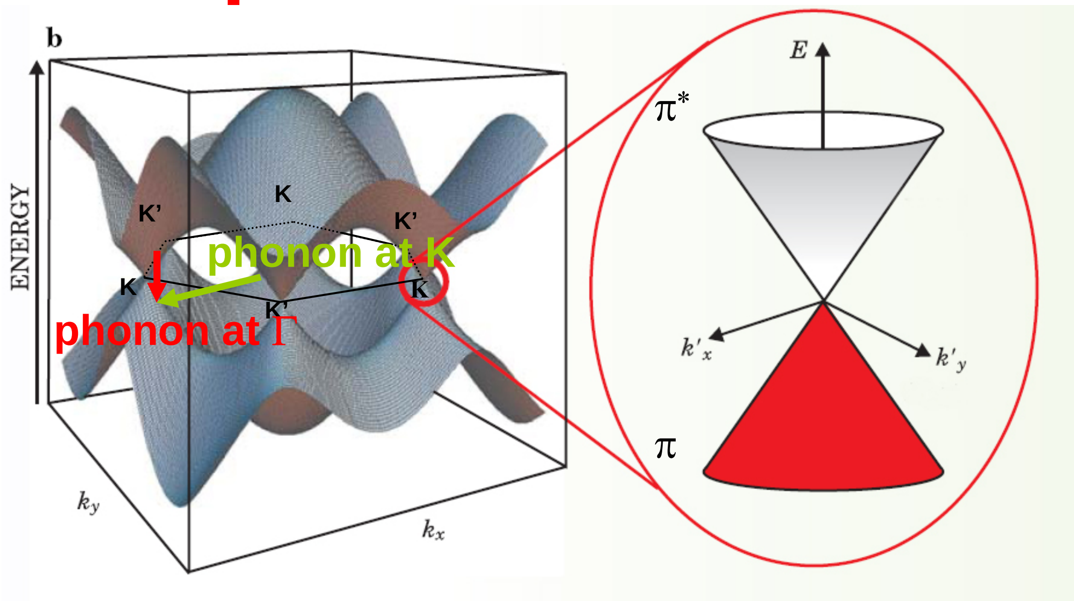
V>0.2 V, non-ballistic regime

- resistance depends on length
- electron scattering length:

10-15 nm

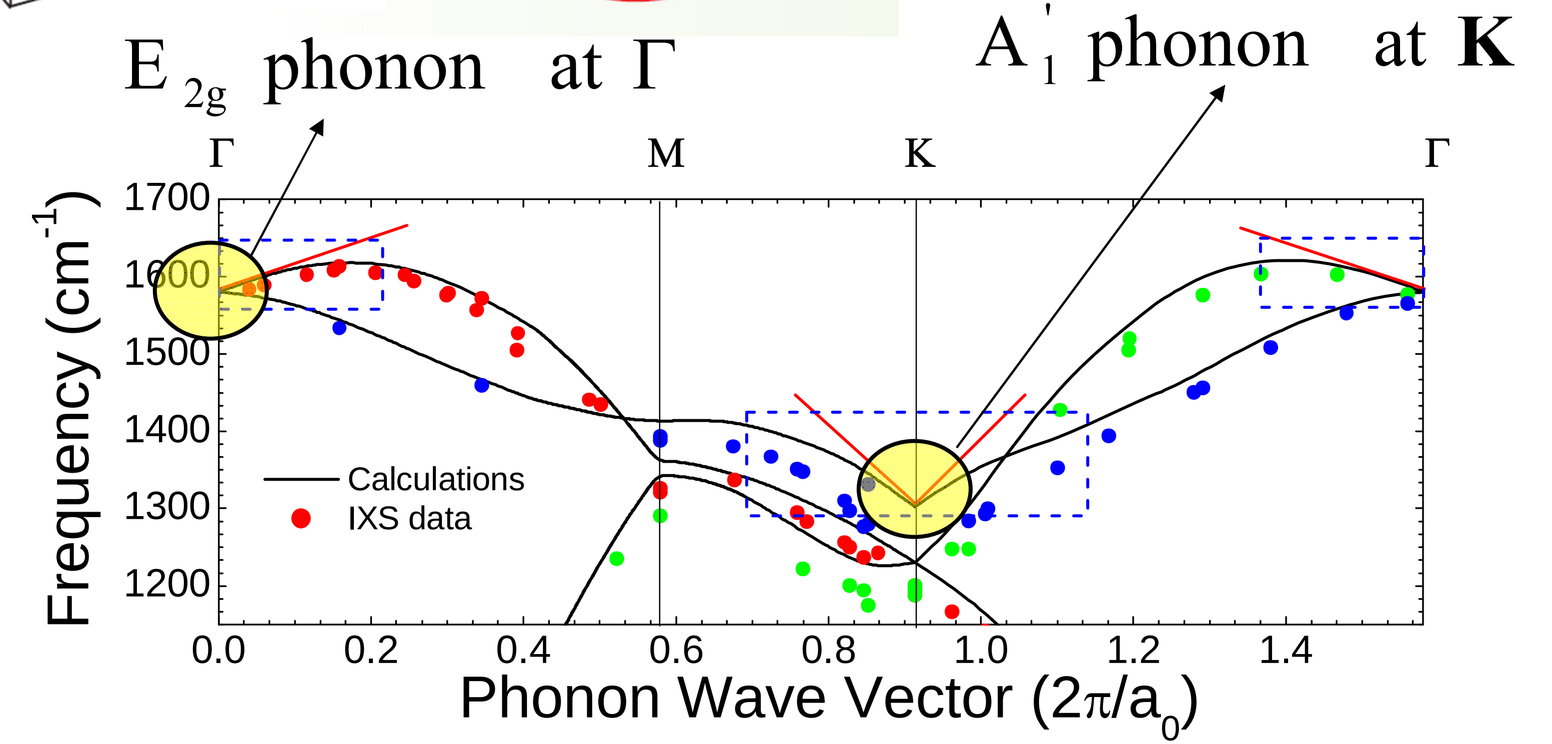
due to optical phonons ~ 0.2 eV

Graphene and tube: electrons and phonons



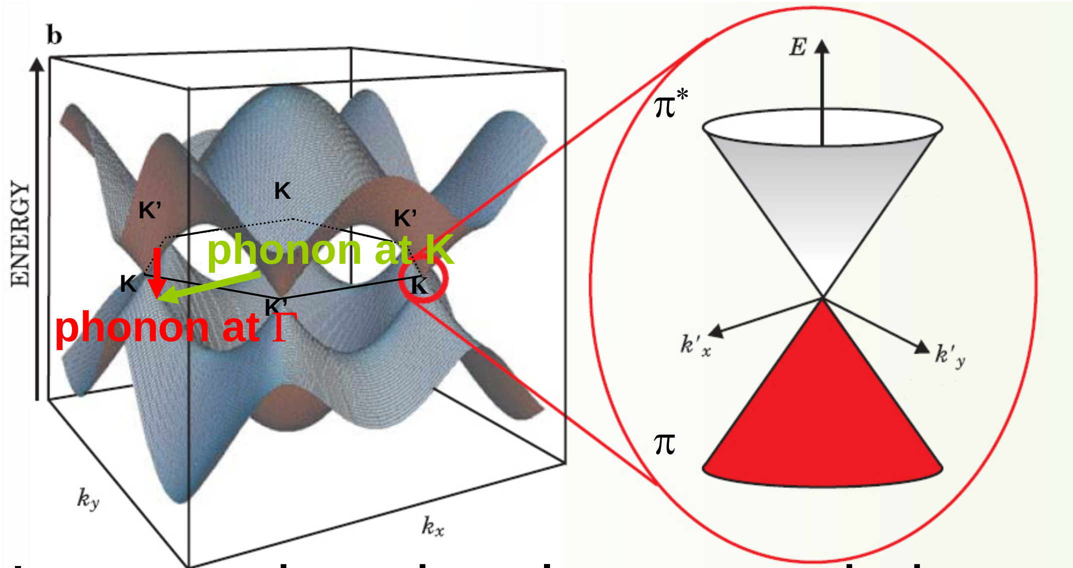
- Fermi surface: circles around **K** and **K'=2K**

- **Optical phonon relevant for transport: Γ and K**

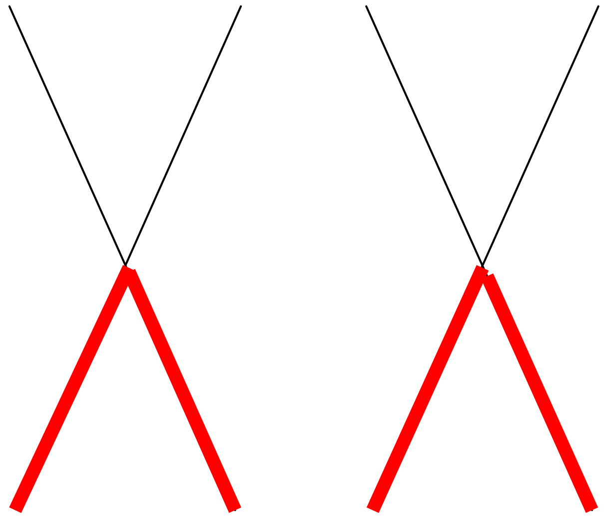


Metallic tubes: electronic structure

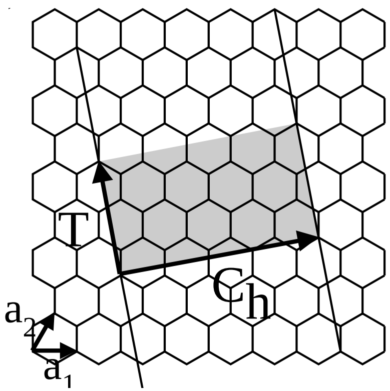
graphene

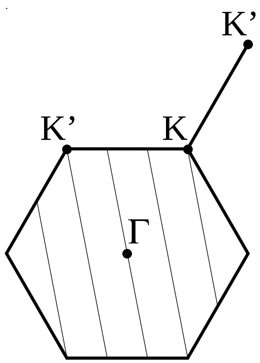


metallic tubes



In nanotubes the electron and phonon states are well described by those of graphene with $\mathbf{k \cdot C_h} = 2\pi$ i, (i integer)



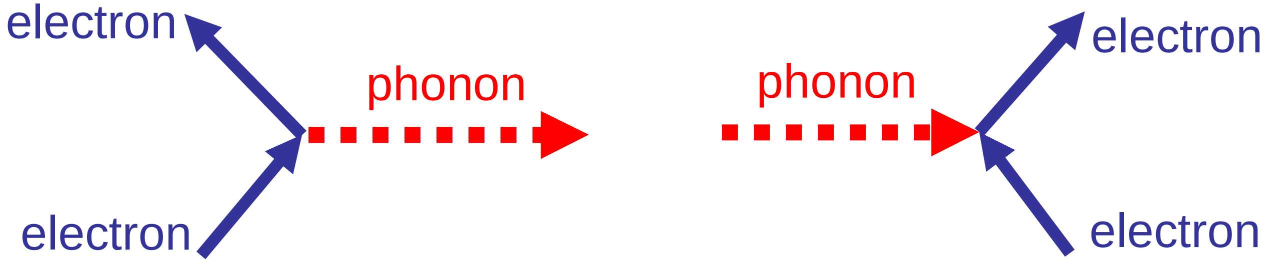


Metallic tubes: (m-n)=3 i, (I integer)

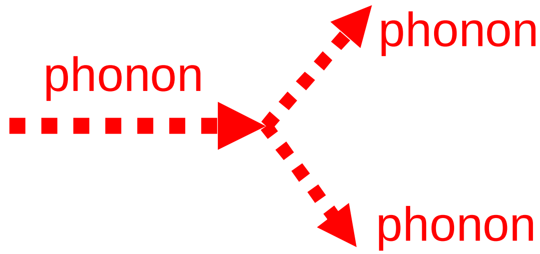
Semicond. tubes:(m-n) $\neq$ 3 i, (i integer)

collision processes for transport

electron-phonon:

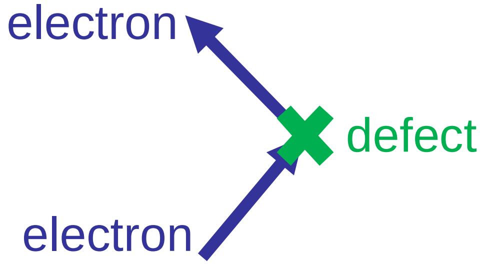


phonon-phonon (anharmonicity):



DFT (GW) calculations, validated with phonon measurements

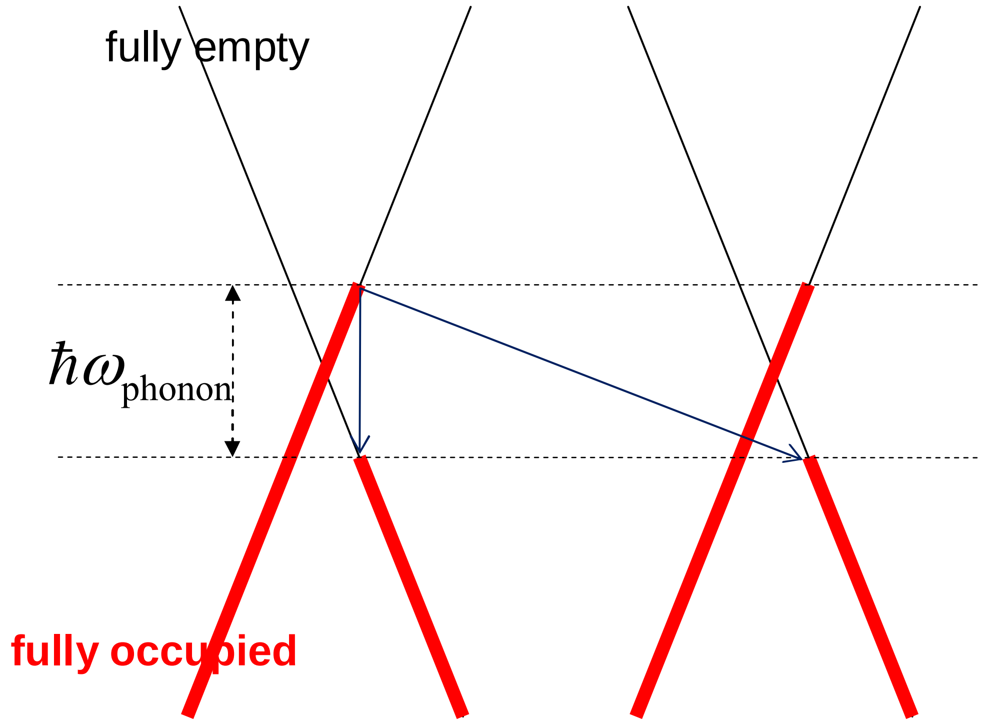
electron-defects (extrinsic):

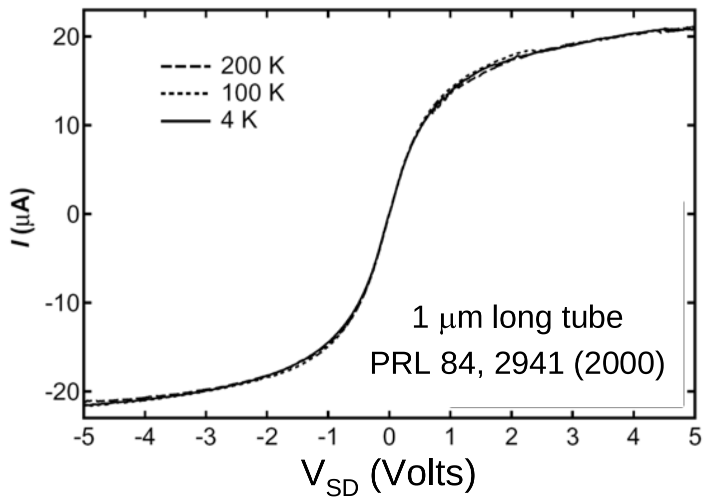


extracted from experimental low-field conductivity

saturation current in tubes

full saturation model





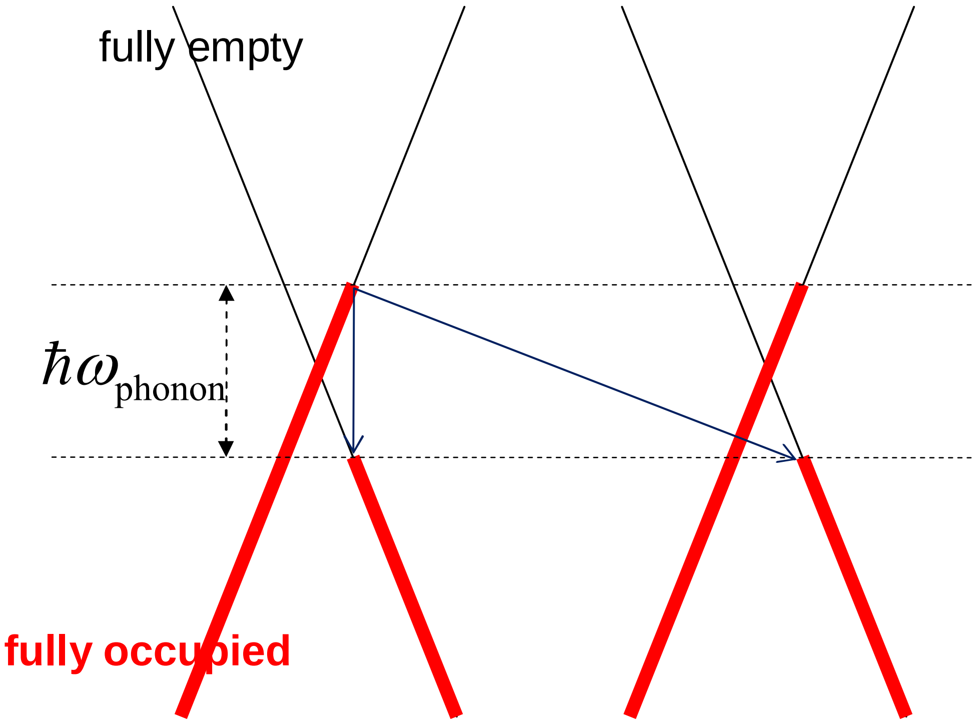
If phonon emission instantaneous once the threshold is reached,(long tubes, V_{sd} not too large)

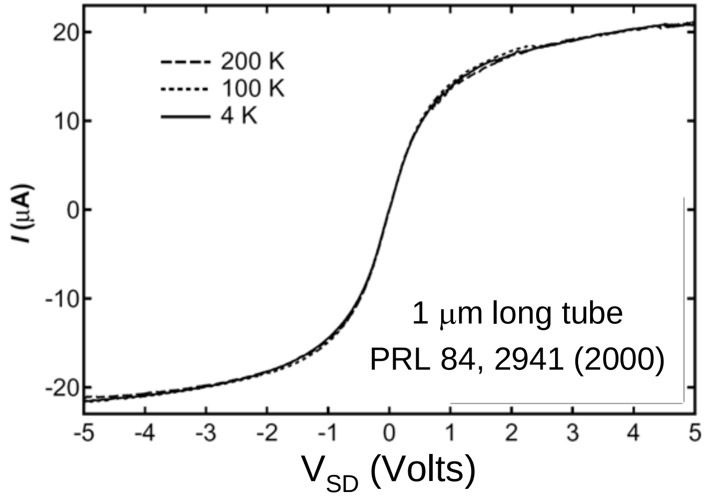
elastic scattering negligible,

$$I = 4\int \frac{dk}{2\pi} e v_k = 4\int \frac{dk}{2\pi} e \frac{d\varepsilon_k}{\hbar dk} = \frac{4e}{2\pi\hbar}\int d\varepsilon = \frac{4e}{2\pi\hbar}\hbar\omega_{\text{phonon}}$$

saturation current in tubes

full saturation model





If phonon emission instantaneous once the threshold is reached,(long tubes, V_{sd} not too large)

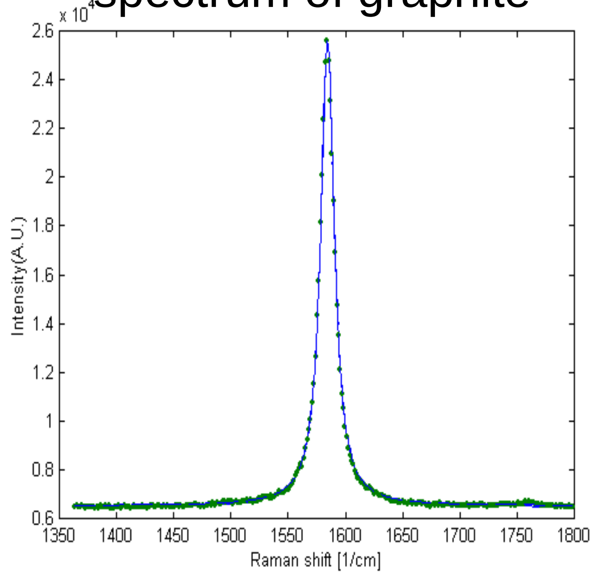
elastic scattering negligible,

$$I = \frac{4e}{2\pi\hbar}\hbar\omega_{\text{phonon}} = 24\mu\text{A}, \quad \text{with} \ \ \hbar\omega_{\text{phonon}} = 0.15\text{meV}$$

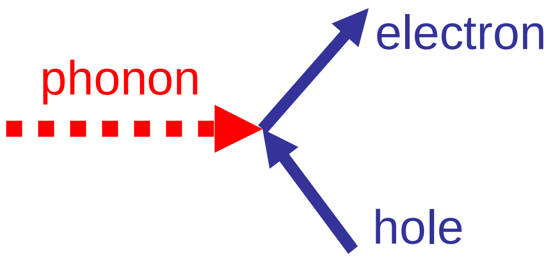
Phonon lifetime in graphite/graphene

[Lazzeri, Piscanec, Mauri, Ferrari, Robertson, Phys. Rev. B 73, 155426 (2006)]

experimental Raman spectrum of graphite



- The Raman G line in graphite E_{2g} phonon at Γ and is well fitted by a Lorenzian with FWHM=13cm^{-1}
- The width is due to the finite lifetime



EPC^2 — hole — electron

$$\text{FWHM} = \gamma_{\vec{q}} = \frac{4\pi}{N_k} \frac{\hbar}{2M\omega_{\vec{q}}} \sum_{k,o,e} \left| \left\langle \vec{k}+\vec{q},e \left| \Delta V_{\vec{q}} \right| \vec{k},o \right\rangle \right|^2 \delta(\varepsilon_{\vec{k},o} - \varepsilon_{\vec{k}+\vec{q},e} + \hbar\omega_{\vec{q}})$$

graphite lattice parameter

$$\gamma_\Gamma = \frac{4\pi^4 \sqrt{3} a^2}{M v_F^2} EPC(\Gamma)^2$$

Fermi velocity

From the Raman G peak line width we can measure EPC

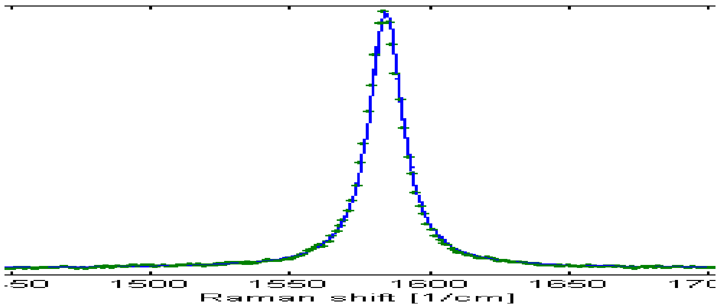
Graphene EPC at Γ

	EPC^2 $(eV/A)^2$
DFT	45.6
Raman line width	45.5

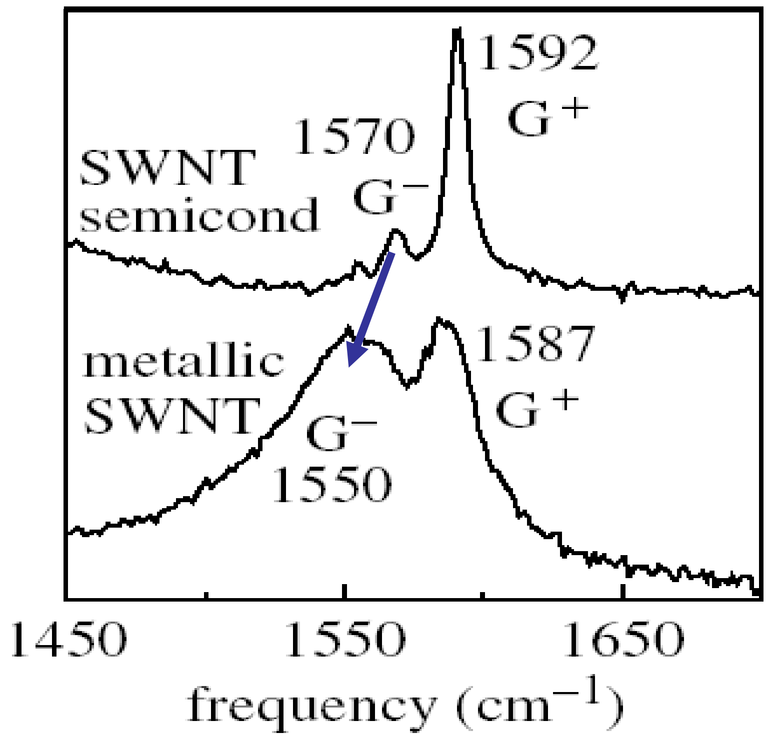
- Similar result from analysis of phonon dispersions near Γ (Kohn anomaly)

Phonon lifetimes in nanotubes

Raman spectrum of graphite



Raman spectrum of tubes



- The G peak splits in G^+ and G^-
- G^- broad and downshifted in metallic tubes

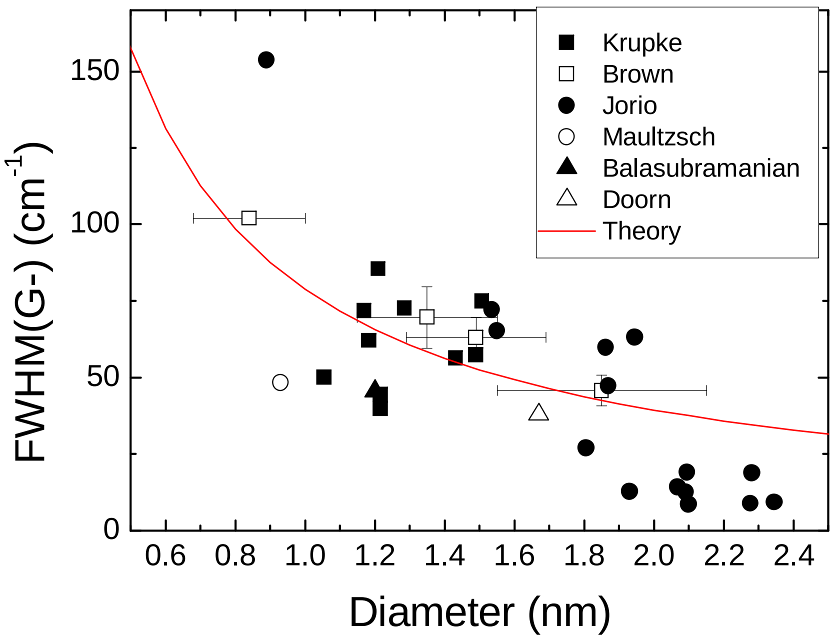
The 2-fold degenerate E_{2g} mode of graphite splits in metallic tubes:

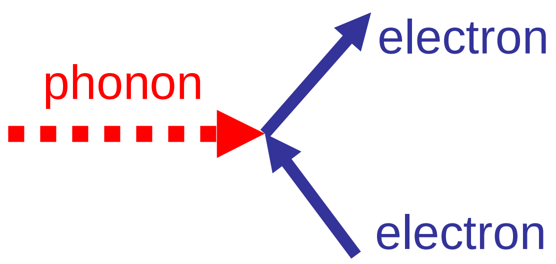
- G+ transverse mode, perp. to the tube axes, not coupled to electrons
- G- longitudinal mode, parall. to the tube axes, coupled to electrons

Raman G peak linewidth in nanotubes

[Lazzeri, Piscanec, Mauri, Ferrari, Robertson, Phys. Rev. B 73, 155426 (2006)]

G$^-$ linewidth in metallic tubes





By using the refolded EPC of graphite:

$$\gamma_{G^+} = 0$$

$$\gamma_{G^-} = \frac{8\pi\sqrt{3}}{M\omega_\Gamma v_F}\frac{a^2}{d}EPC(\Gamma)^2 = \frac{79[\text{cm}^{-1}\text{nm}]}{d}$$

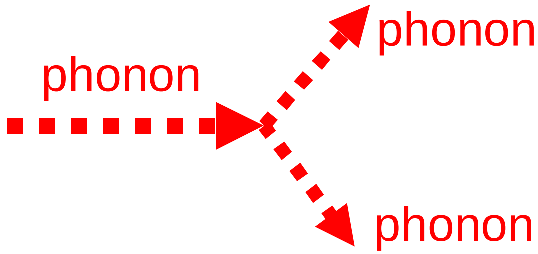
graphite lattice parameter

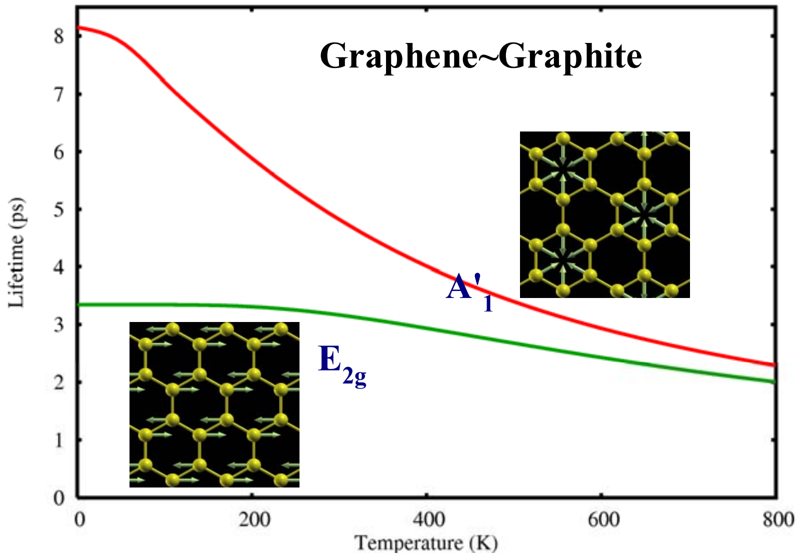
graphite EPC

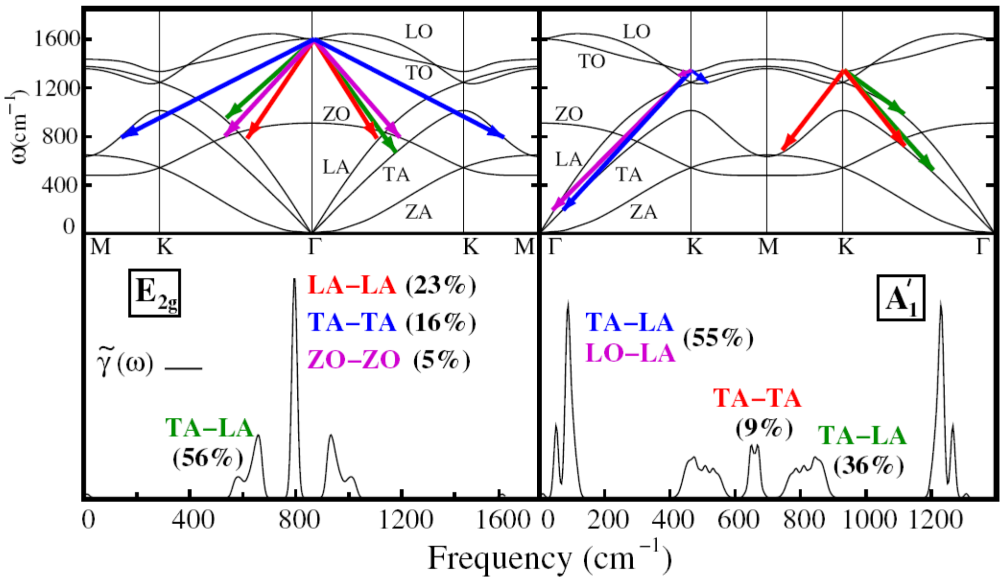
tube diameter

phonons-phonons (anharmonicity) interaction from DFT

[Bonini, Lazzeri, Marzari, Mauri, Phys. Rev. Lett. 99, 176802 (2007)]

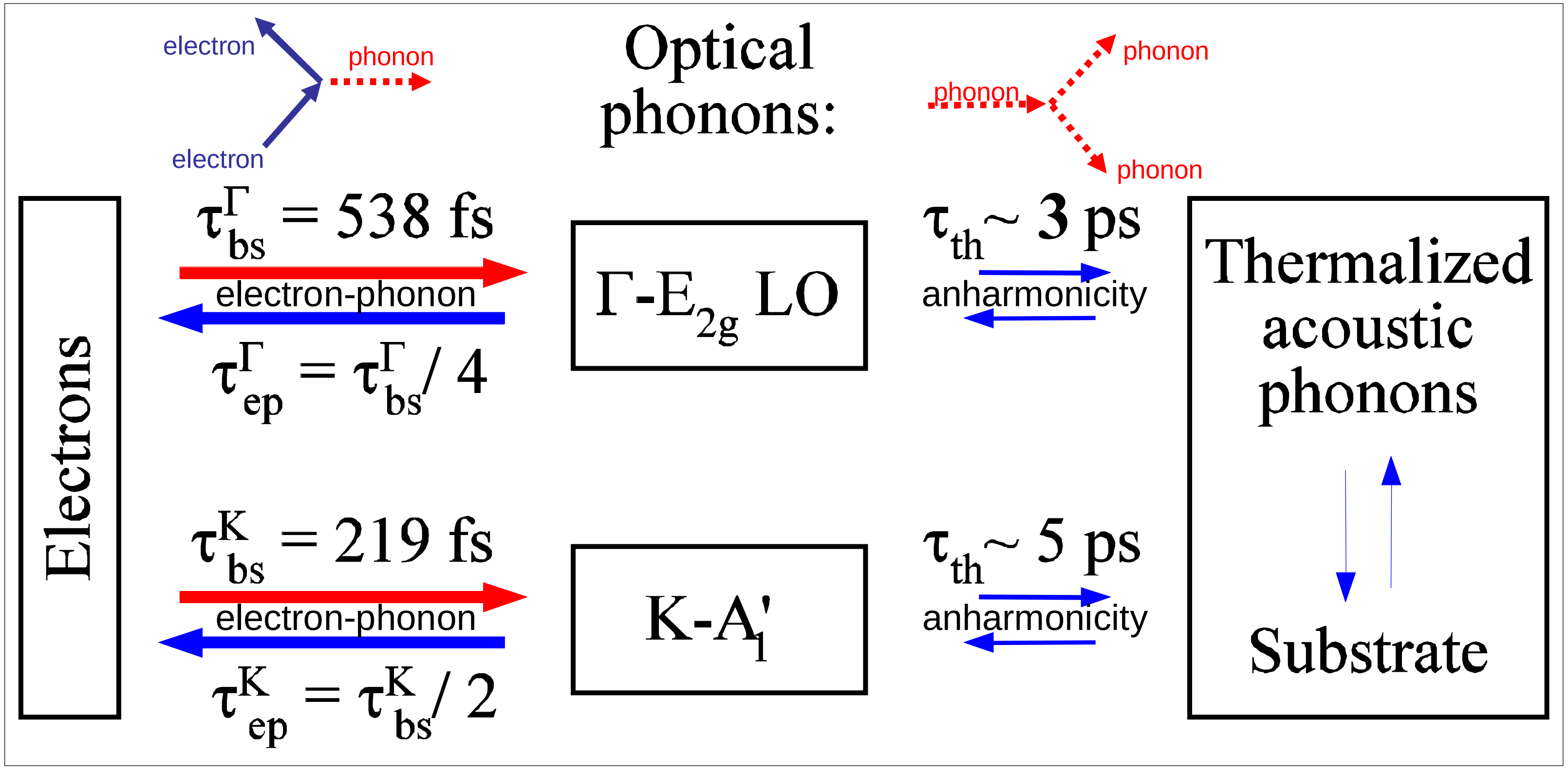






Time resolved terahertz spectroscopy [PRL 95, 187403 (05)] on graphite: $\tau_{\text{anharmonic}} \sim 7\text{ps}$

Scattering times for nanotubes with a diameter of 2 nm



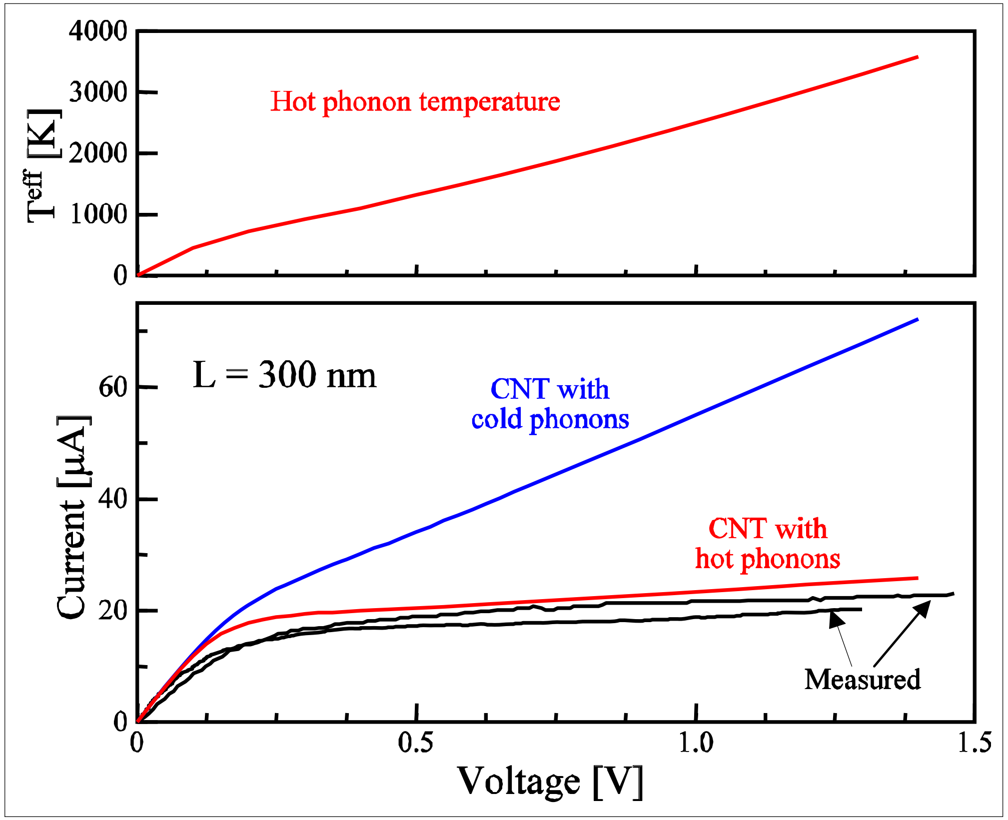
- bottleneck: relaxation from optical to acoustic phonon
- heating of optical phonons is expected

We use the scattering times in Boltzmann semiclassical transport theory for both electrons and phonons

[Lazzeri, Mauri, Phys. Rev. B 165419 (2006)]

- We compute the IV curve of metallic nanotube transistors with:
  - cold phonons: supposing that optical phonons are thermalized at room temperature
  - hot phonons: allowing for the possibility that optical phonons are heated by the electrons

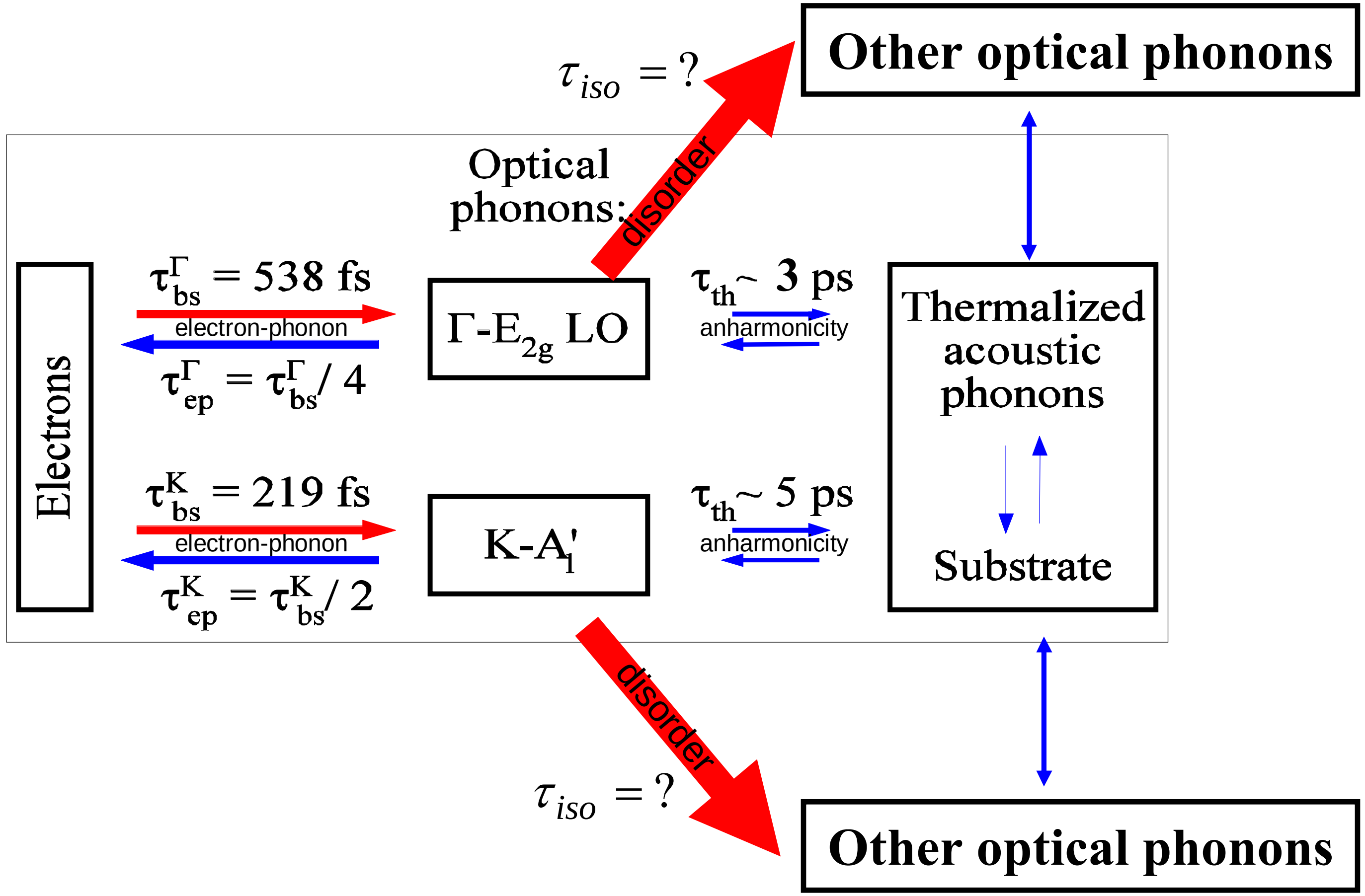
results (300 nm long nanotube)



- under transport optical phonons are very hot
- other phonons (non coupled to electrons) are cold: tube *not in thermal equilibrium*!
- we can boost performances with a heat sink

a heat sink: isotopic disorder $^{12}C_x{}^{13}C_{1-x}$

[Vandecasteele, Lazzeri, Mauri, **102**, 196801 (2009)]

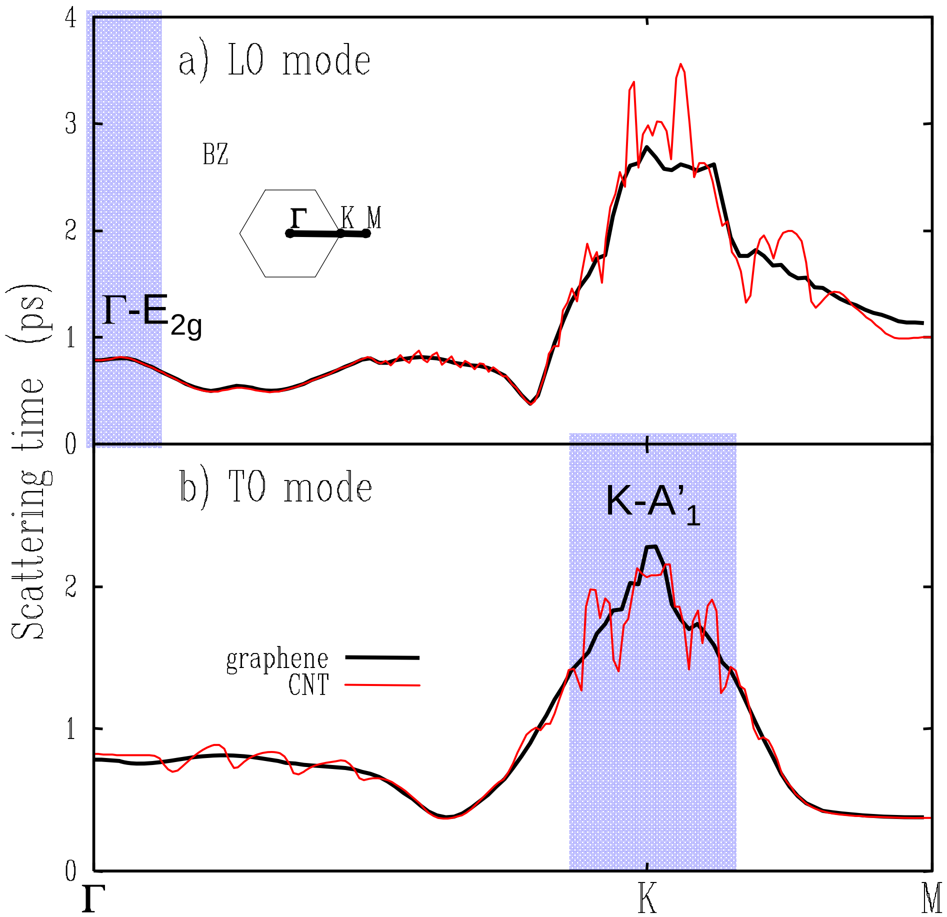


- isotopic disorder scatters phonons but not electrons
- is the disorder-decay-time shorter than τ_{th} (3-5 ps)?

a heat sink: isotopic disorder $^{12}C_x{}^{13}C_{1-x}$

[Vandecasteele, Lazzeri, Mauri, **102**, 196801 (2009)]

with x=0.5



$\tau_{iso} \sim 0.9\text{ps} < 3\text{ps} = \tau_{th}$

$\tau_{iso} \sim 2\text{ps} < 5\text{ps} = \tau_{th}$

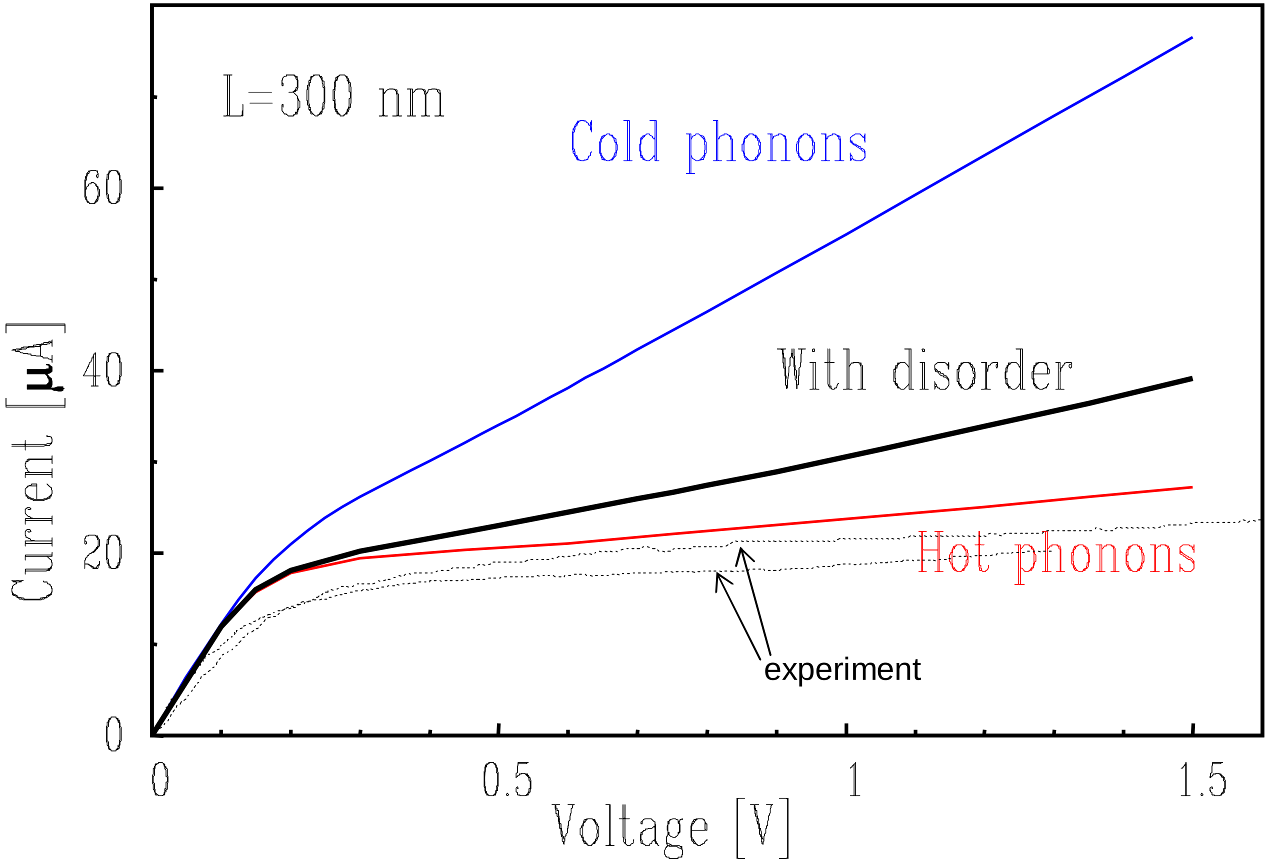
- is the disorder-decay-time shorter than τ_{th} (3-5 ps)?

yes

a heat sink: isotopic disorder $^{12}C_x{}^{13}C_{1-x}$

[Vandecasteele, Lazzeri, Mauri, **102**, 196801 (2009)]

with x=0.5



- improvement in the performances (decrease of differential resistivity)

Conclusions part 1

metallic carbon nanotubes

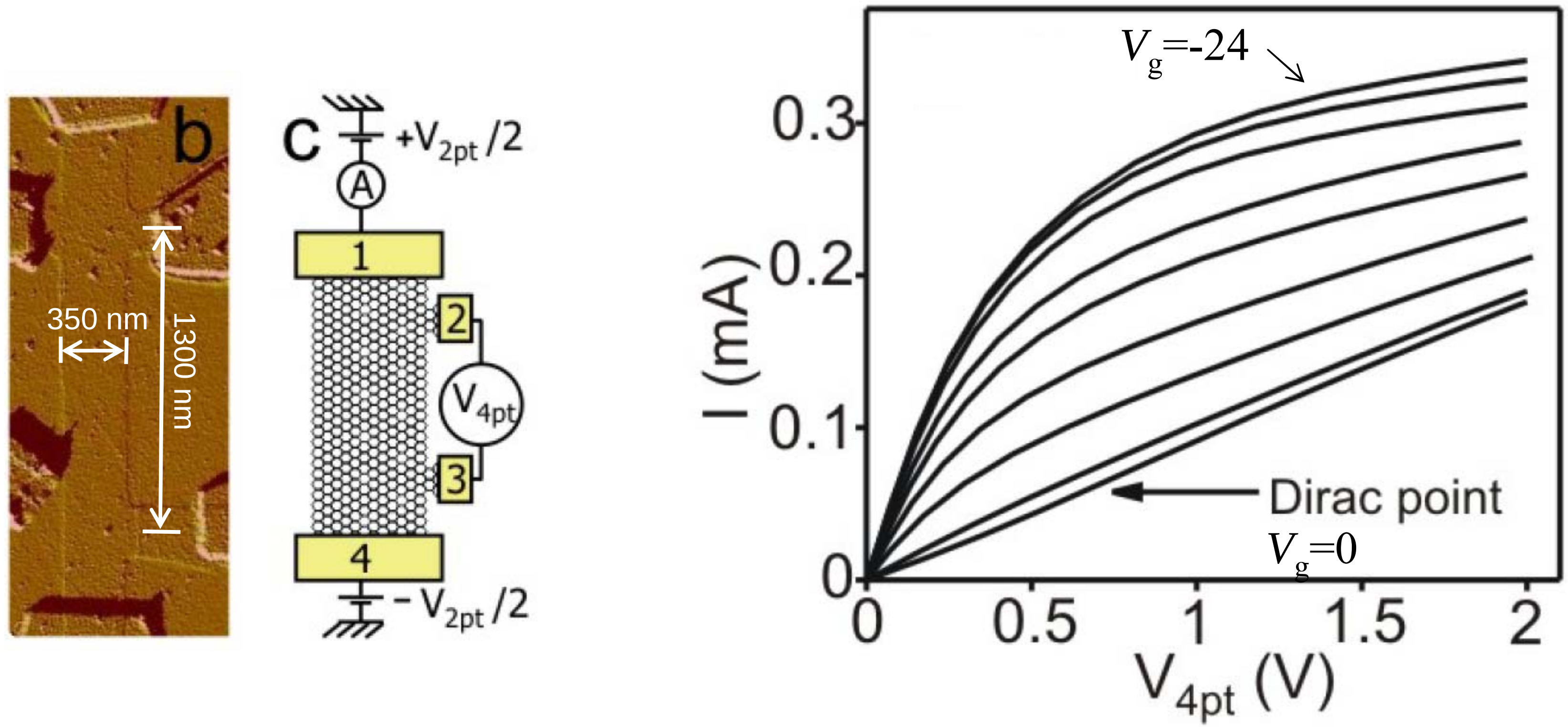
- full saturation is possible, since l_{el} ~ 1000 nm >> l_{ph} ~ 100 nm
- at high bias, since $\tau_{epc} << \tau_{anharmonic}$, phonons become hot and increase the resistance
- isotopic disorder reduces the hot phonons and the resistance

PART 2:

Transport at high field in doped graphene

graphene at high bias in high mobility samples ($\sim 10^4 cm^2V^{-1}s^{-1}$)

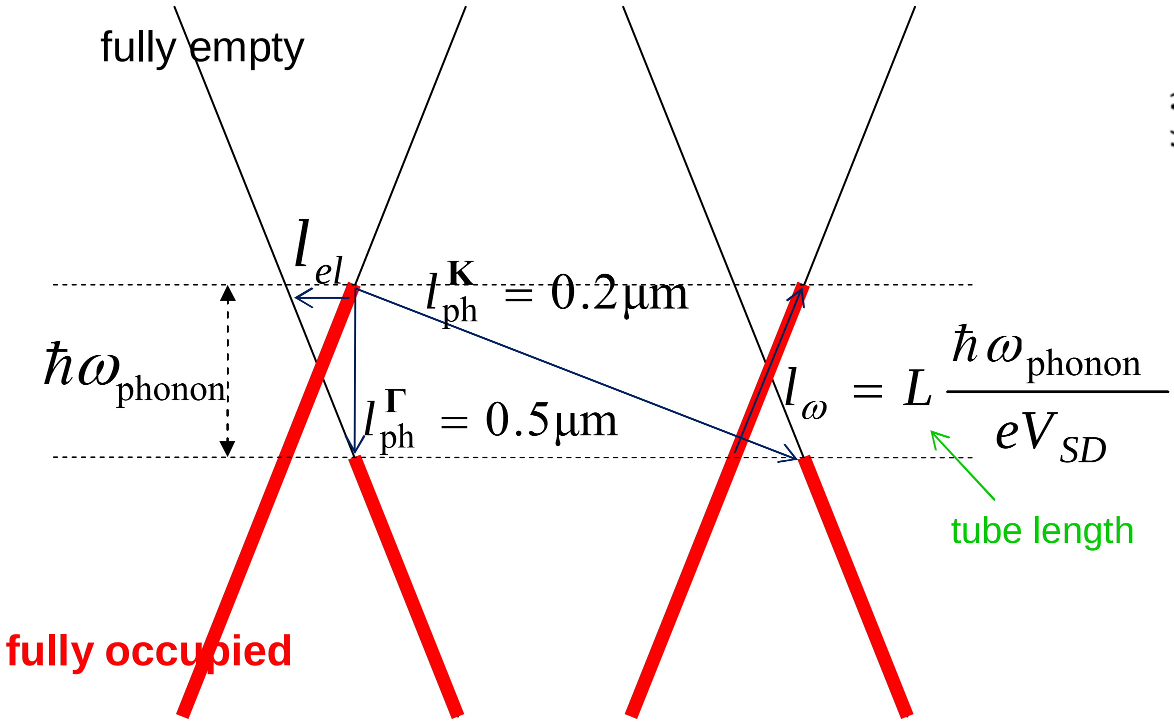
[Barreiro,Lazzeri,Moser,Mauri,Bachtold, PRL **103**, 076601 (2009)]

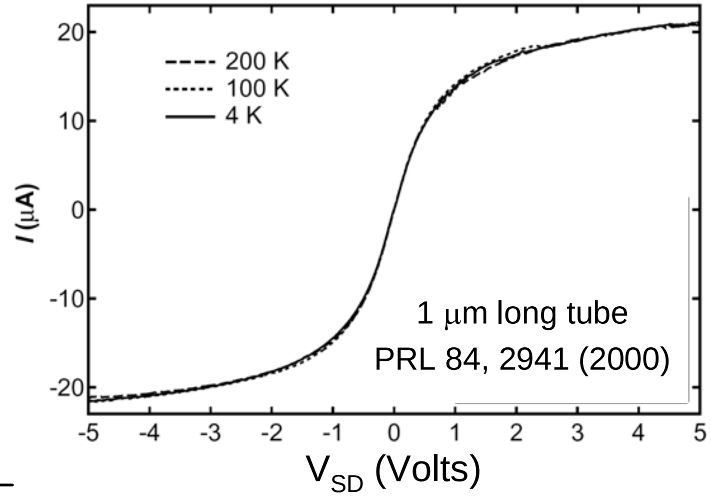


- differential resistance increases by current never fully saturates
- current 350μA/350nm ~ 1 μA/nm. In nanotubes 20μA/(π2nm) ~ 3μA/nm

tube: saturation current

full saturation model





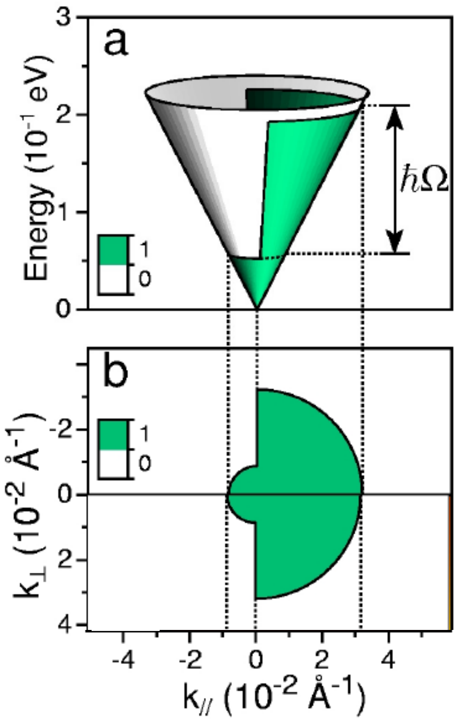
If phonon emission instantaneous once the threshold is reached,
$l_{ph} << l_\omega$ (long tubes) and
elastic scattering negligible, $l_{el} << l_{ph}$ (from expt. $l_{el} \sim 1.6\mu m$)

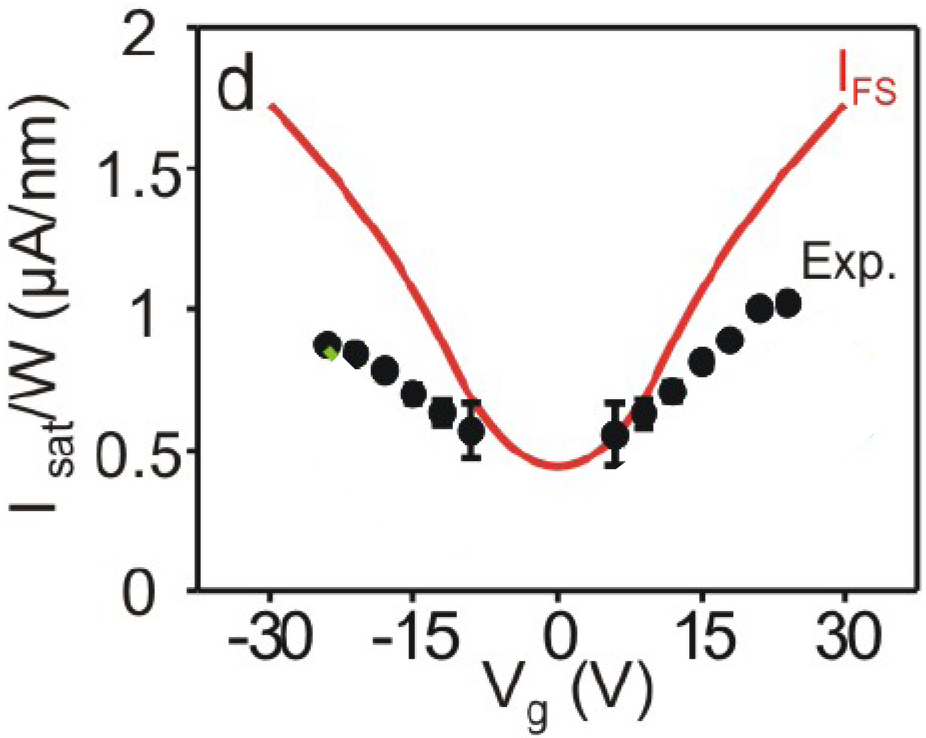
$$I = \frac{4e}{2\pi\hbar}\hbar\omega_{phonon} = 24\,\mu A, \quad \text{with} \quad \hbar\omega_{phonon} = 0.15\,\text{meV}$$

graphene: saturation current

[Barreiro,Lazzeri,Moser,Mauri,Bachtold, PRL **103**, 076601 (2009)]

full saturation model





•if phonon emission instantaneous once the threshold is reached and elastic scattering negligible

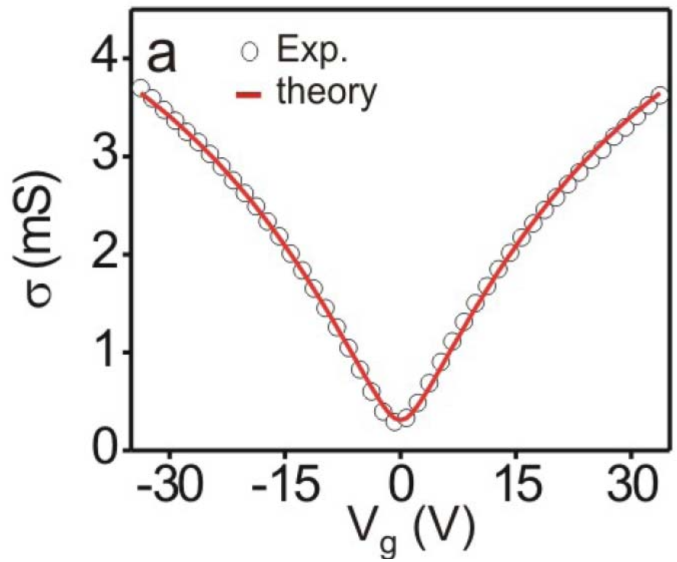
•this model overestimates the current in graphene

Boltzmann theory for electrons and phonons

[Barreiro,Lazzeri,Moser,Mauri,Bachtold, PRL **103**, 076601 (2009)]

•intrinsic parameters: electron-phonon and phonon-phonon (anharmonic) scattering length from DFT (and GW) calculations

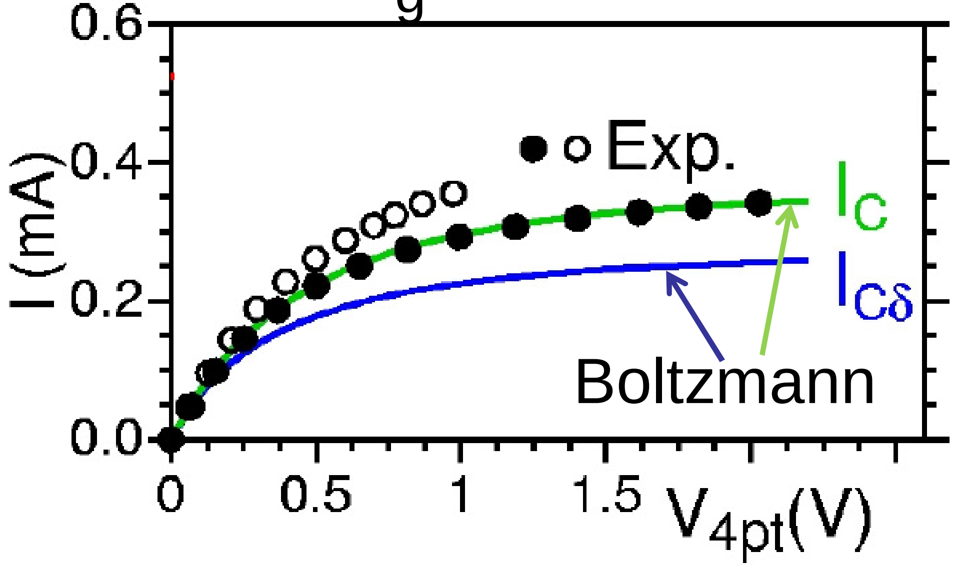
•extrinsic parameters: elastic scattering length modeled as in [Hwang, Das Sarma, PRB 77, 195412 (2008)]**.** Free parameters (density of charged and neutral defects) fitted to reproduce the low-bias experimental conductivity. Two models (C and Cδ) equally good at low bias.



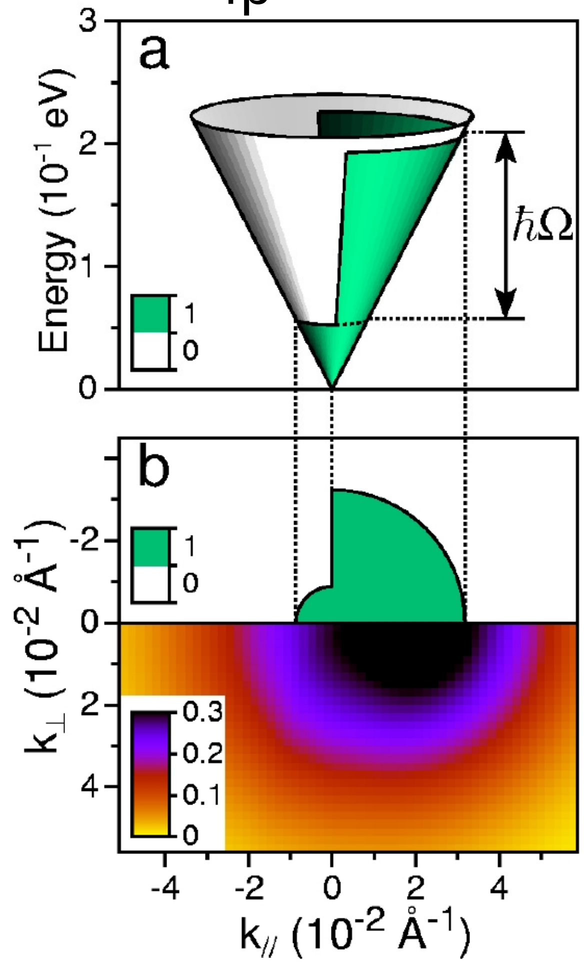
Boltzmann theory for electrons and phonons

[Barreiro,Lazzeri,Moser,Mauri,Bachtold, PRL **103**, 076601 (2009)]

V_g=+-24V



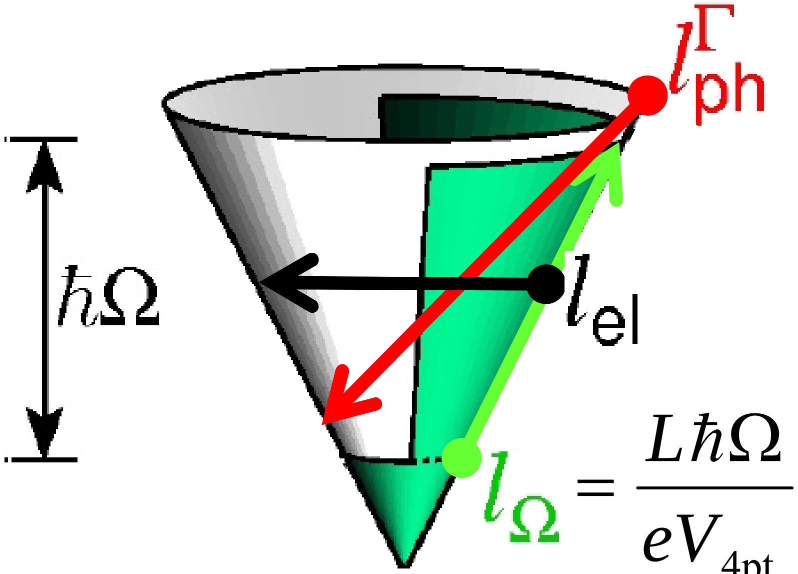
V_{4p}=2V

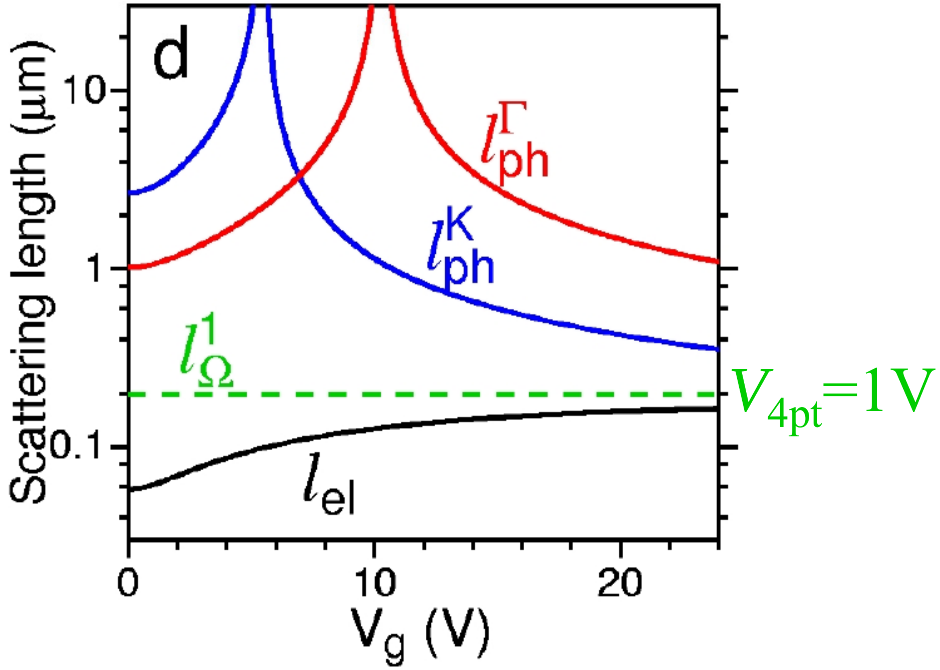


- Boltzmann reproduces partial saturation seen in expt.
- no hot phonon (optical phonons thermalized with other phonons), but we do not exclude self-heating [Nanolett. 9, 1833 and 10,466]
- electron distribution different from full saturation

Scattering lengths in graphene

[Barreiro,Lazzeri,Moser,Mauri,Bachtold, PRL **103**, 076601 (2009)]

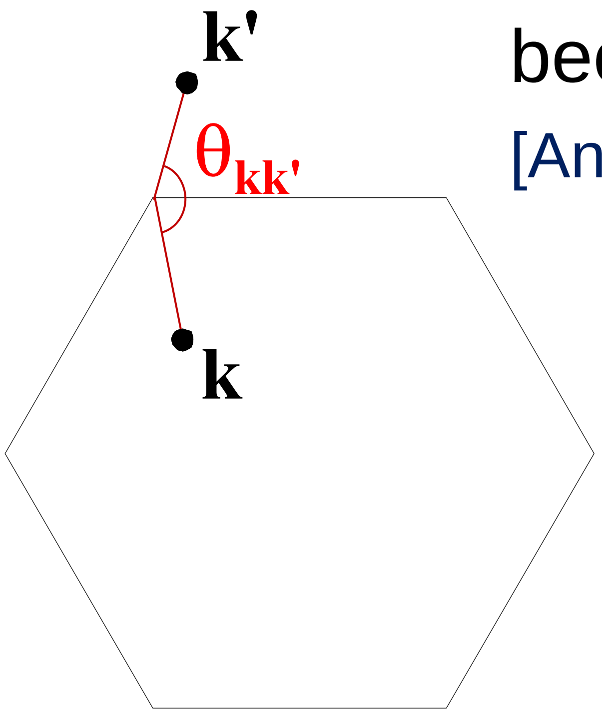




•saturation starts for the value of V_{4pt} for which $l_{\Omega} = l_{el}$

•saturation is complete if the phonon emission is instantaneous, $l_{ph} << l_{\Omega}$, and the elastic scattering is negligible, $l_{\Omega} << l_{el}$. This is impossible in graphene since $l_{el} << l_{ph}$

why is the elastic scattering more important in graphene than in tubes?

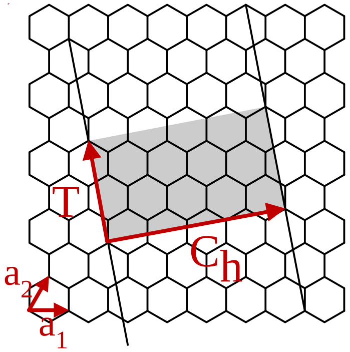


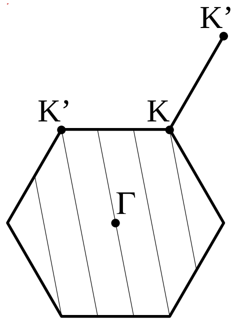
because of pseudospin conservation

[Ando et al., J. Phys. Soc. Jpn. 67, 2857 (1998)]:

$$\text{scattering} \propto \left|V(\mathbf{k}-\mathbf{k}')\right|^2 \cos^2(\theta_{\mathbf{kk}'}/2)$$
$$= 0 \quad \text{if} \quad \theta_{\mathbf{kk}'} = \pi$$

in metallic nanotubes $\theta_{\mathbf{kk}'}=\pi$





Conclusions part 1 & 2

metallic carbon nanotubes

- full saturation is possible, since l_{el} ~ 1000 nm >> l_{ph} ~ 100 nm
- at high bias, since $\tau_{epc} << \tau_{anharmonic}$, phonons become hot and increase the resistance
- isotopic disorder reduces the hot phonons and the resistance

graphene

- no full saturation, since l_{el} ~ 100 nm << < l_{ph} ~ 600 nm
- current per lateral length 1μA/nm no hot-phonons since elastic
- scattering challenges and reduces the electron-phonon scattering
- higher currents are possible by reducing l_{el} or by increasing V_g

PART 3:

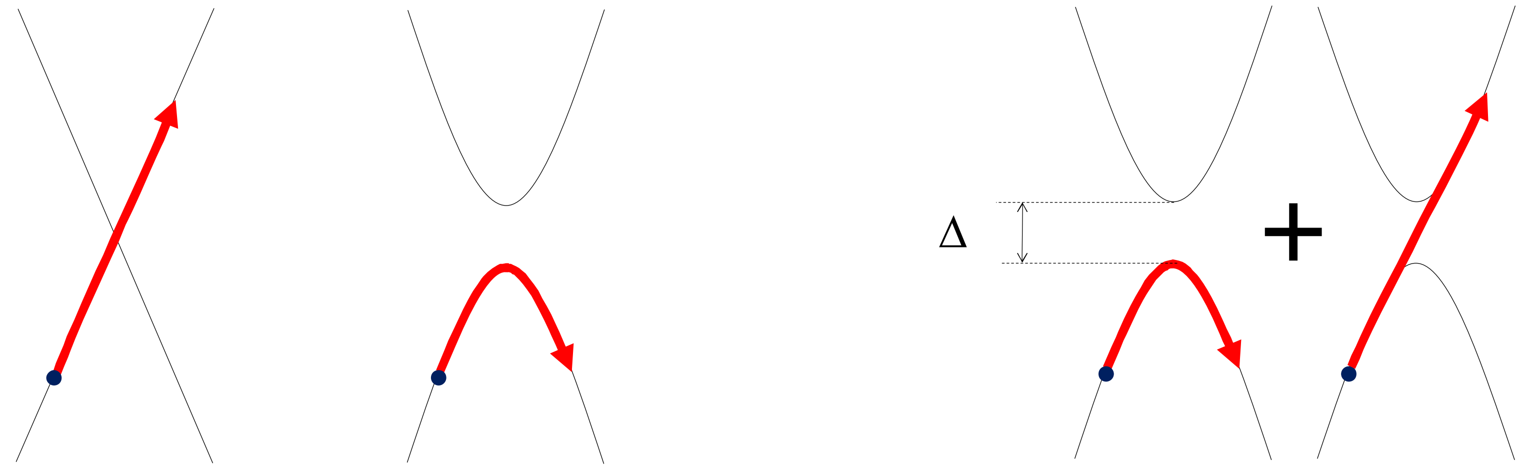
Transport at high field near the charge neutrality point

Zener (Klein) tunneling in tubes

semi-classical
(Boltzmann)

full-quantum
Zener

metallic semicond. semicond.



Andreev PRL 99, 247204 (2007)

tunneling probability

$$T = \exp\left(-\frac{\pi\Delta^2}{4\hbar v_F e E}\right)$$

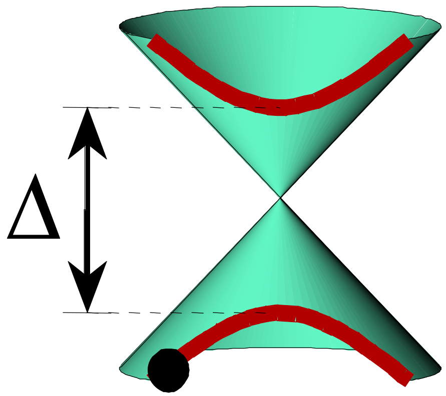
source-drain electric field

sizable for

$$E = \frac{\pi\Delta^2}{4\hbar v_F e} \sim 300\ \frac{\text{Volt}}{\mu\text{m}} \quad (\text{for}\ \ \Delta = 0.5\text{eV})$$

Zener (Klein) tunneling in graphene

$$\hbar \frac{d\mathbf{k}}{dt} = -e\mathbf{E} \qquad k_{\perp} = \text{constant}$$

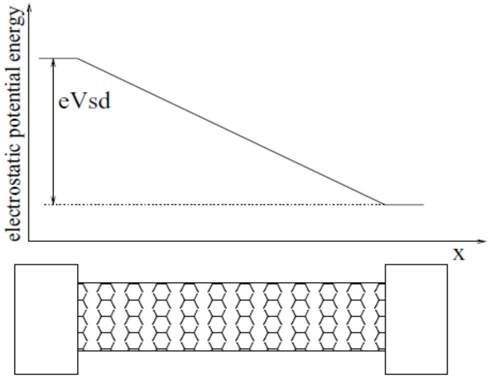


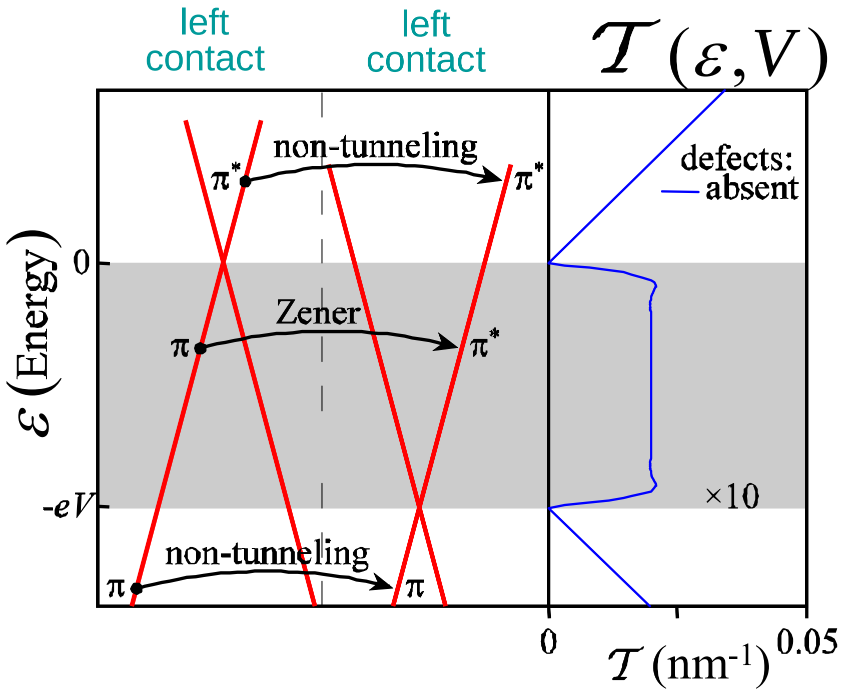
$$\Delta = 2\hbar v_{\mathrm{F}} k_{\perp}$$

Zener tunneling is present for any value of the electric field

Zener tunneling in graphene: ballistic

transmission (per lateral length) along a 1μm long graphene channel with TB model and Non-Equilibrium Green-functions





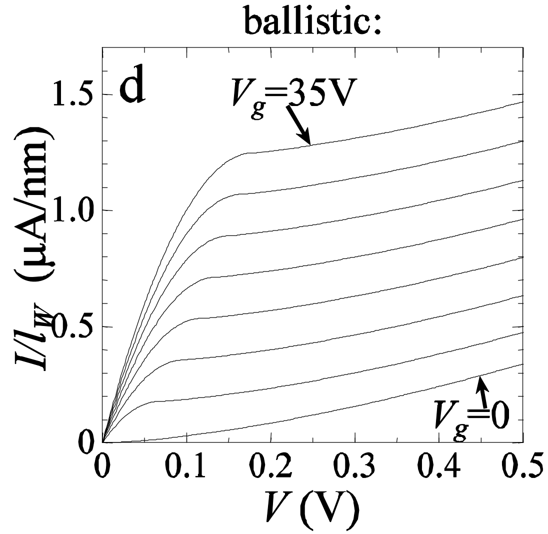
$$\mathcal{T}(\varepsilon, V) = \int \frac{dk_\perp}{2\pi} T(\varepsilon, k_\perp, V)$$

= transmission from

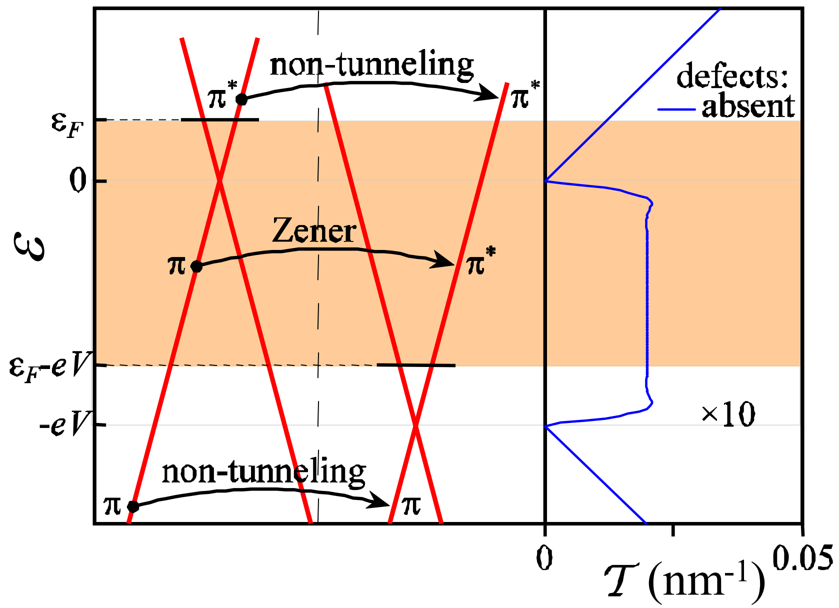
the left- to the right-contact

Zener tunneling in graphene: ballistic

electric current (I)
per lateral length (l_w)



$$\frac{I(V)}{l_w} = \frac{4e}{2\pi\hbar}\int_{\varepsilon_F - eV}^{\varepsilon_F} d\varepsilon\, \mathcal{T}(\varepsilon, V)$$

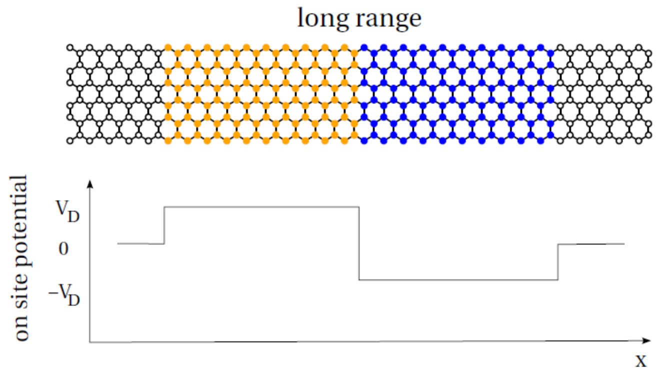


-with $V_g=0$ ($\varepsilon_F=0$) only Zener

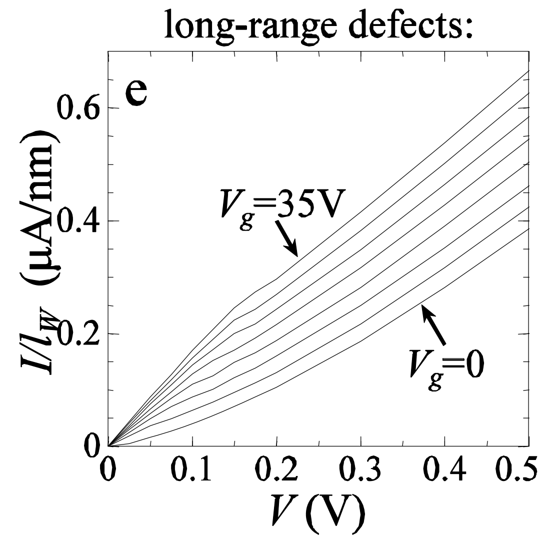
$$I \propto V^{1.5}$$

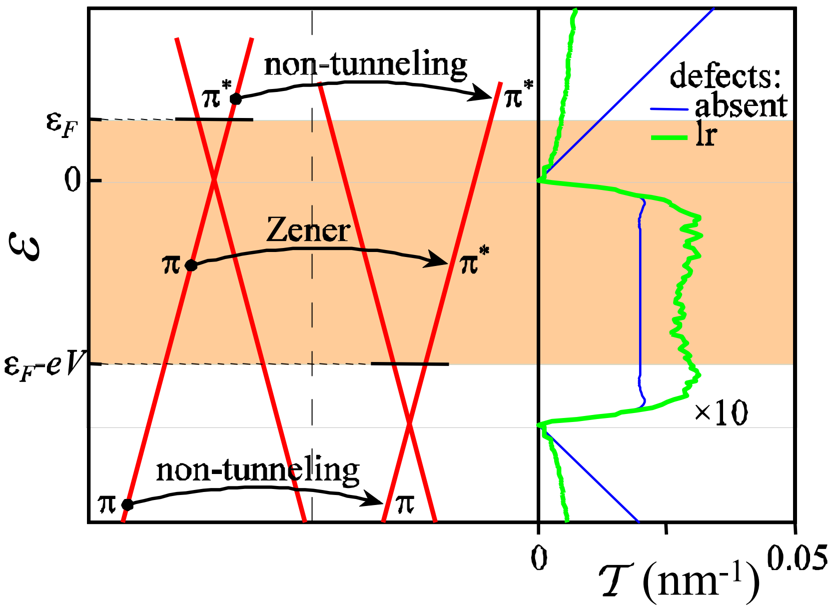
-with $V_g>5\text{Volt}$ ($\varepsilon_F>0$) non-tunneling current dominates

Zener tunneling in graphene with defects



$$\frac{I(V)}{l_w} = \frac{4e}{2\pi\hbar}\int_{\varepsilon_F - eV}^{\varepsilon_F} d\varepsilon\, \mathcal{T}(\varepsilon, V)$$





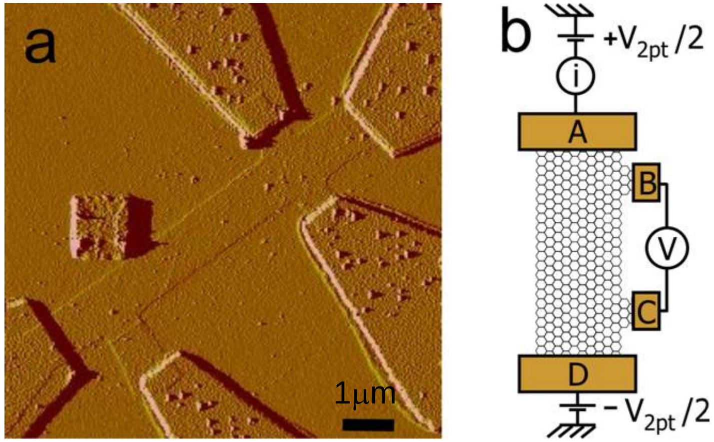
-defects kill the non-tunneling current but enhance the Zener one

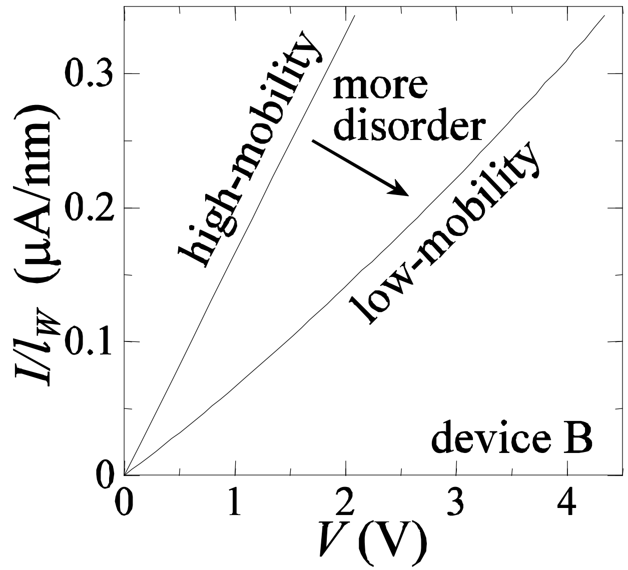
-now even at finite doping

$$I \propto V^{\alpha} \quad \text{with} \quad \alpha > 1$$

Zener tunneling in graphene experiment

Undoped sample (V_g=0)





-high mobility sample (μ=7000cm^{2}V^{-1}s^{-1})

$$I \propto V$$

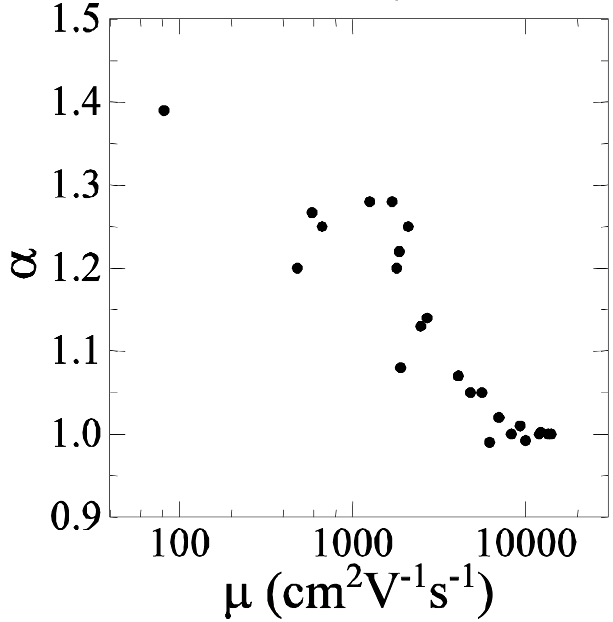
-after 10KeV e-bombardment: low mobility (μ=260cm^{2}V^{-1}s^{-1})

$$I \propto V^{1.2}$$

Zener tunneling in graphene experiment

22 undoped devices (V_g=0)
exponent α vs. mobility

$$I \propto V^{\alpha}$$

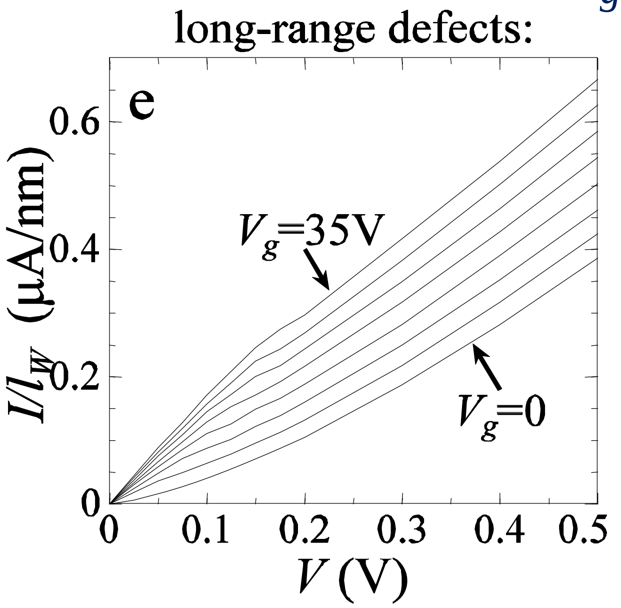


Zener tunneling in graphene experiment

theory

long-range defects

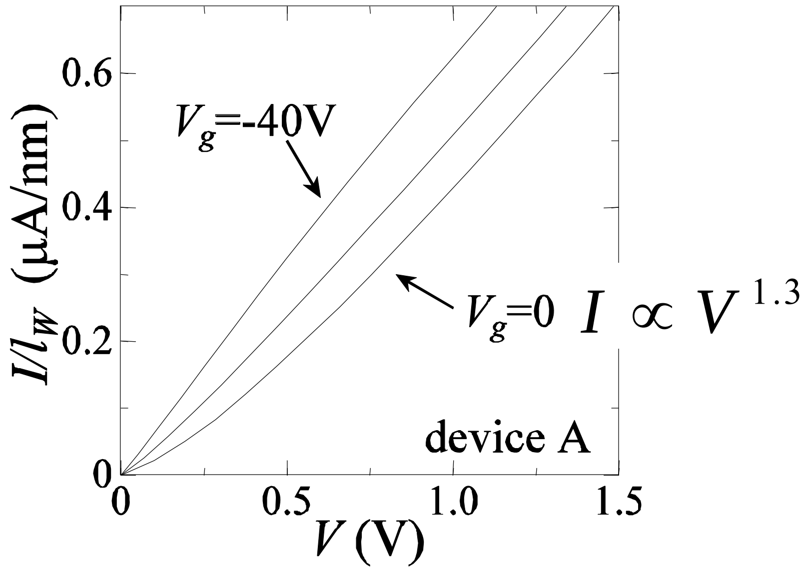
as a function of V_g



experiment

low-mobility (μ=1700cm^{2}V^{-1}s^{-1})

as a function of V_g



conclusions part 2 [PRL **103**, 076601 (2009)]

- in graphene, no full saturation, since l_{el} ~ 100 nm << l_{ph} ~ 600 nm
- no hot-phonons since elastic scattering challenges and reduces the electron-phonon scattering
- current per lateral length 1μA/nm
- higher currents are possible by reducing l_{el} or by increasing V_g

conclusions part 3 [arXiv:1003.2072]

- in high mobility (ballistic) samples the transport is dominated by Zener tunneling only at the exact charge neutrality point

- in low mobility (disordered) samples defects reduce (filter) the non-tunneling current and made visible the Zener tunneling also at finite (low) doping