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

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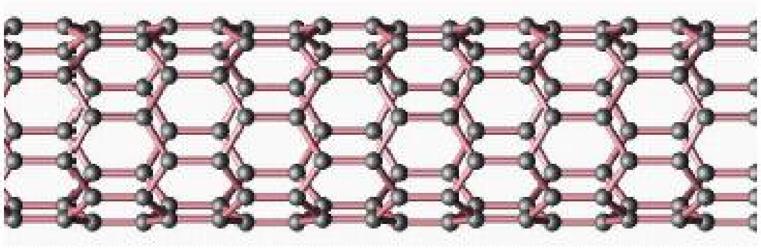
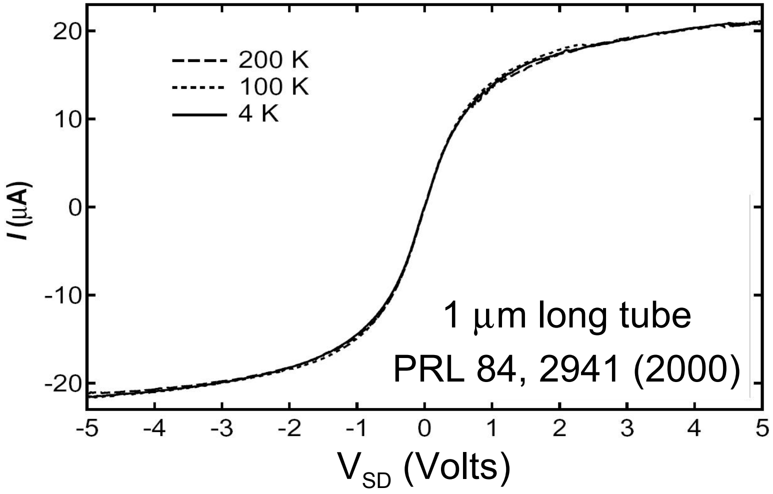
Motivations





Metallic Carbon nanotubes:

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

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

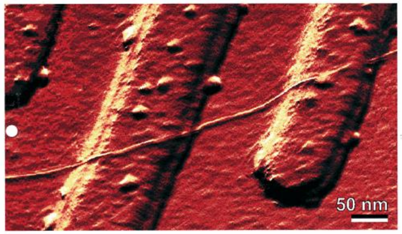
- What is the origin of the saturation?
- Can we improve the nanotube performances?
- Graphene at high bias: maximum current density? Graphene interconnects?

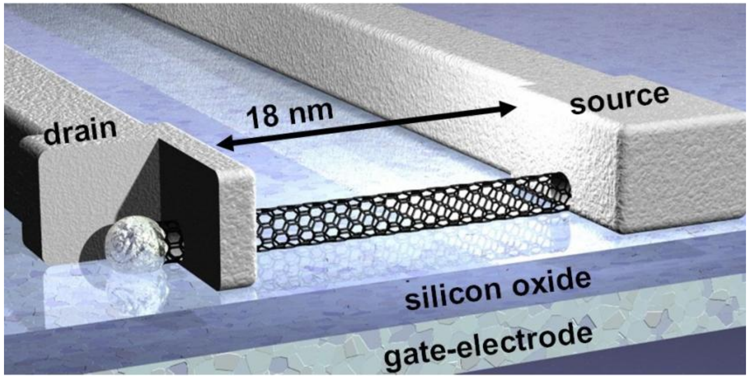
OUTLINE

- 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

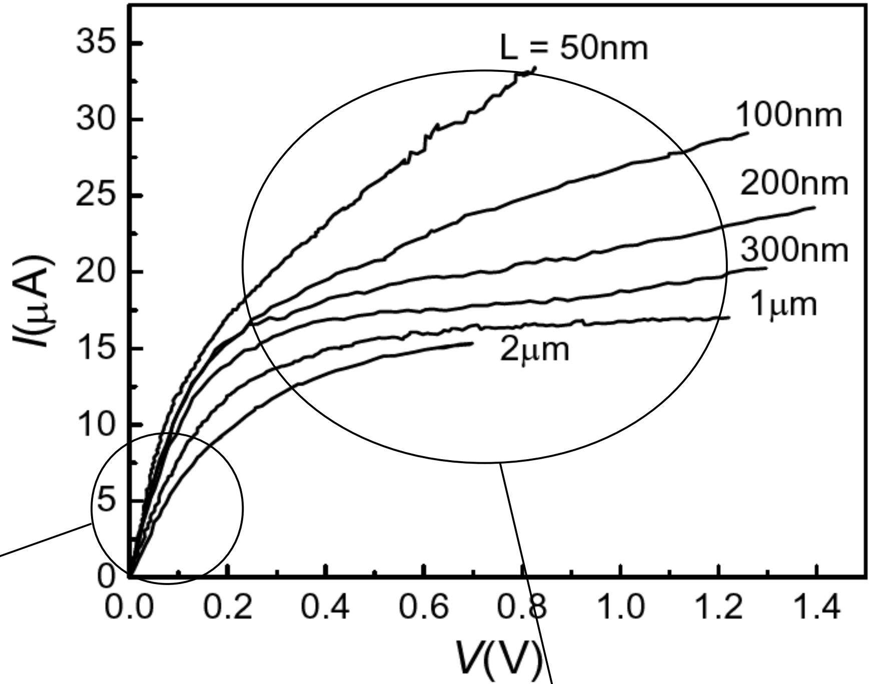
metallic tubes on substrate





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

V>0.2 V, non-ballistic regime

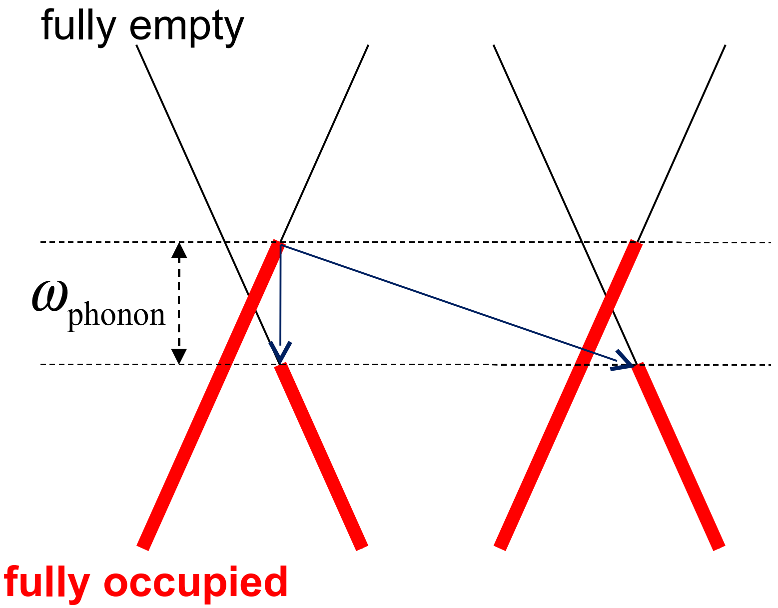
- resistance depends on length
- electron scattering length:

10-15 nm

due to optical phonons ~ 0.2 eV

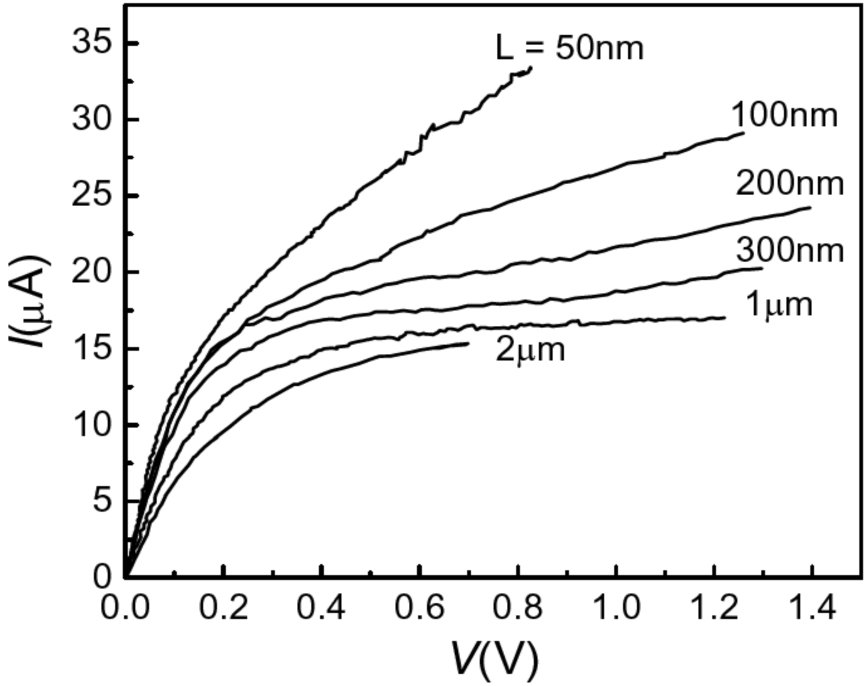
saturation current

full saturation model



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

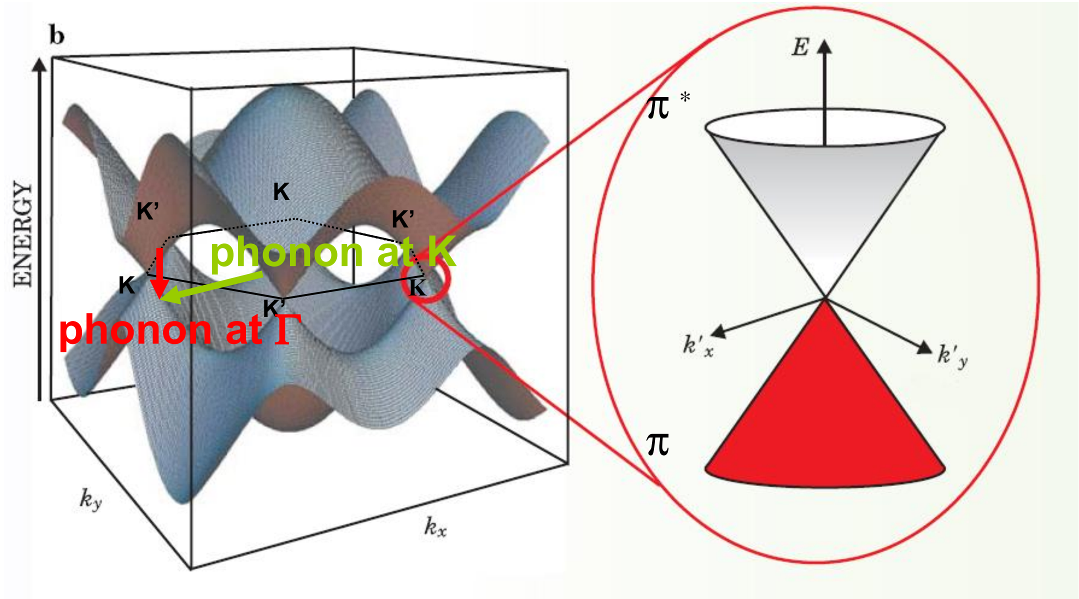
Experimental I/V of a nanotube transistor



If phonon emission instantaneous once the threshold is reached (long tubes) and elastic scattering negligible

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

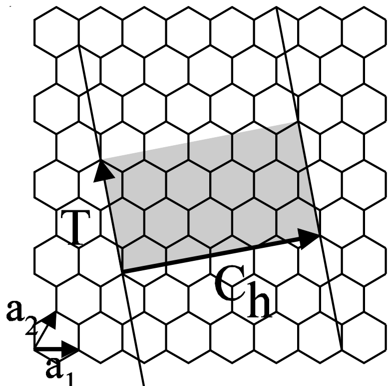
Graphene and nanotube electronic structure

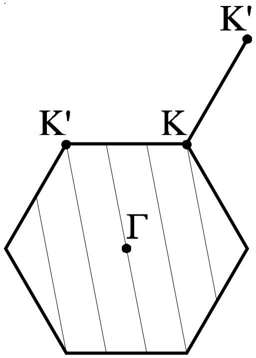


- Fermi surface: circles around **K** and **K**'=2**K**

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

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





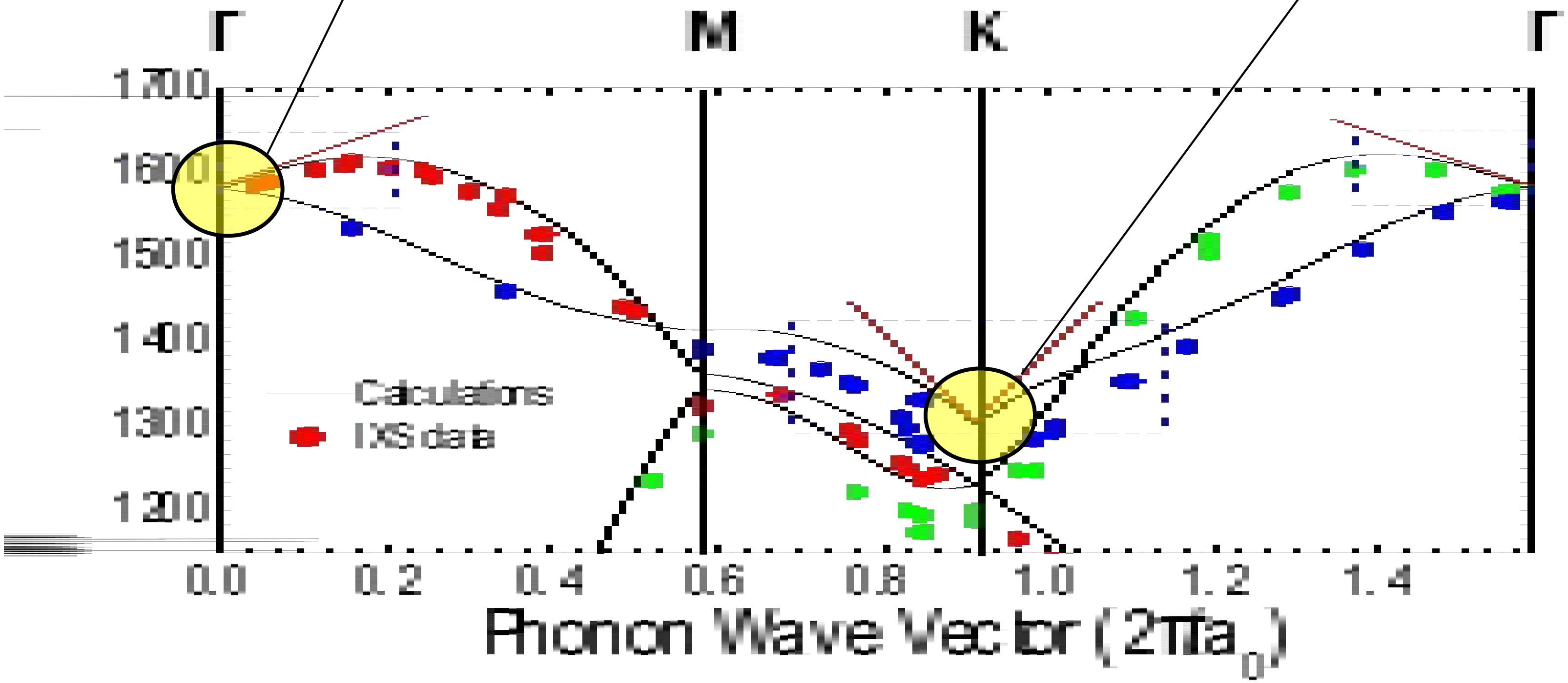
Metallic tubes: (m-n)=3 i, (I integer)

Semicond. tubes:(m-n) ≠ 3 i, (i integer)

optical phonons of graphite/graphene coupled with electrons

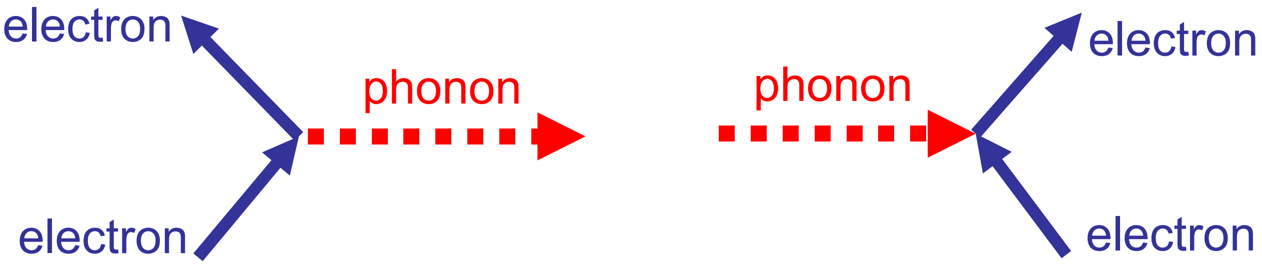
E_{2g} phonon at Γ

A_1' phonon at $\mathbf{K}$

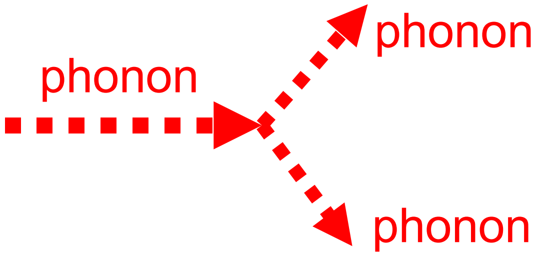


collision processes for transport

electron-phonon:

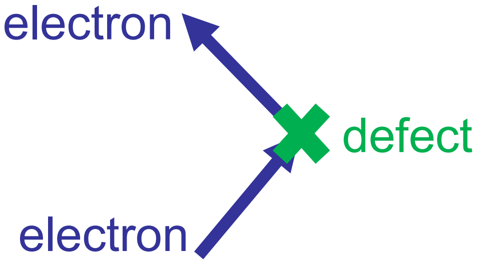


phonon-phonon (anharmonicity):



DFT calculations, validated with phonon measurements

electron-defects (extrinsic):

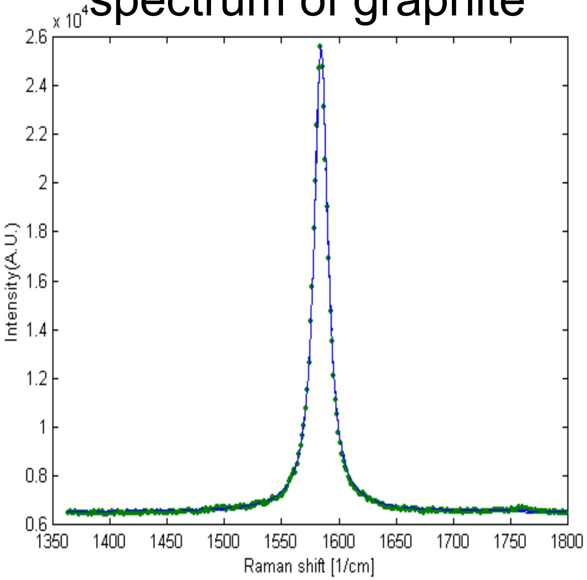


extracted from experimental low-field conductivity
(negligible in nanotubes but not in graphene)

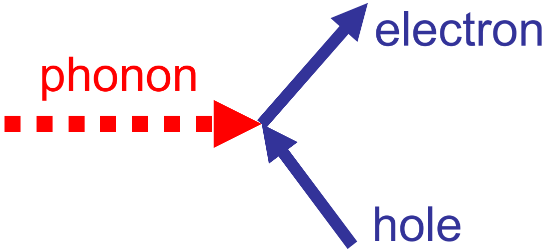
Phonon lifetime in graphite/graphene

[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



EPC²

hole

electron

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

graphite lattice parameter

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

Fermi velocity

From the Raman G peak line width we can measure EPC

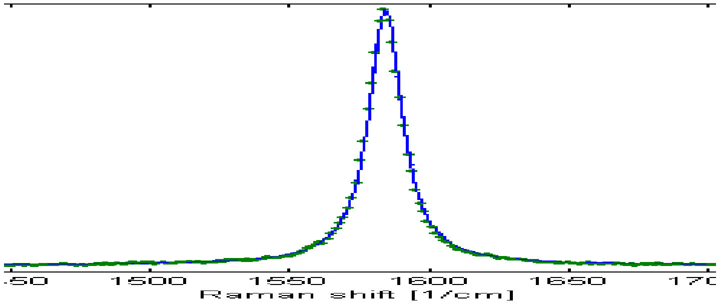
Graphene EPC at Γ

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

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

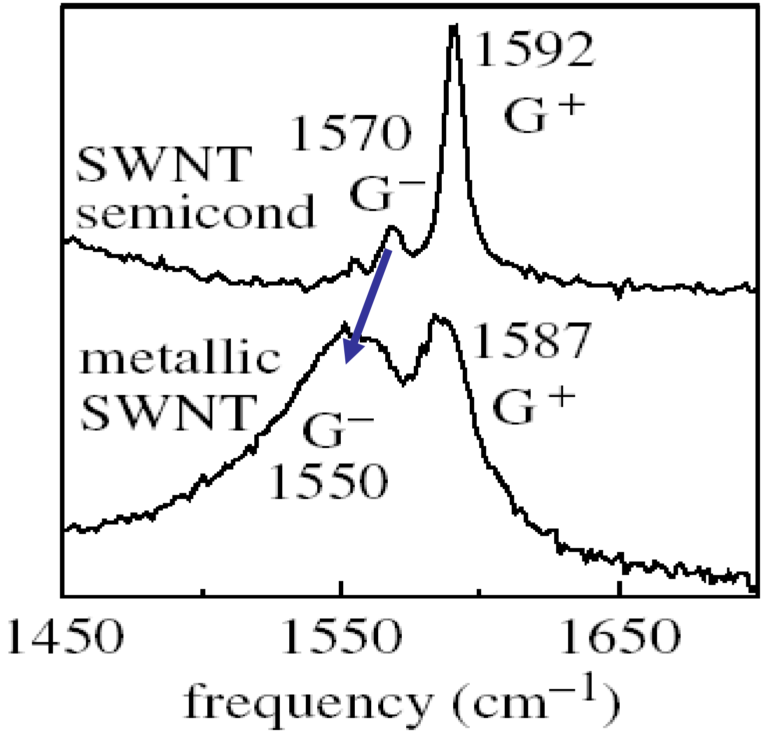
Phonon lifetimes in nanotubes

Raman spectrum of graphite



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

Raman spectrum of tubes



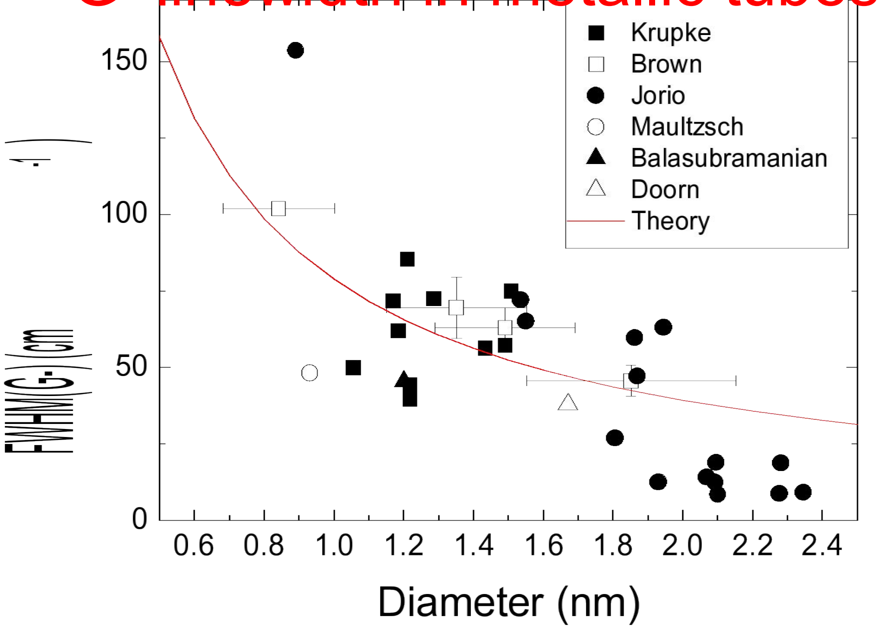
The 2-fold degenerate E_{2g} mode of graphite splits in metallic tubes:

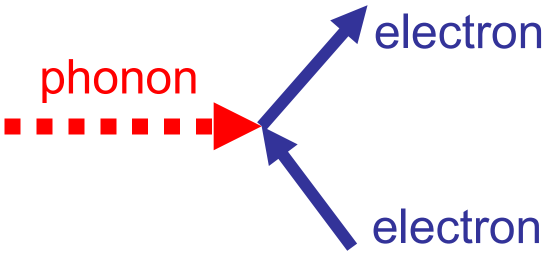
- G+ transverse mode, perp. to the tube axes, not coupled to electrons
- G- longitudinal mode, parall. to the tube axes, coupled to electrons

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:

graphite lattice parameter

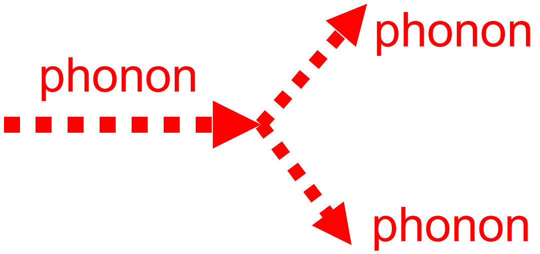
$$\gamma_{G^+} = 0 \qquad \gamma_{G^-} = \frac{8\pi\sqrt{3}}{M\omega_\Gamma v_F}\frac{a^2}{d}EPC(\Gamma)^2 = \frac{79[\mathrm{cm}^{-1}\mathrm{nm}]}{d}$$

graphite EPC

tube diameter

phonons-phonons (anharmonicity) interaction from DFT

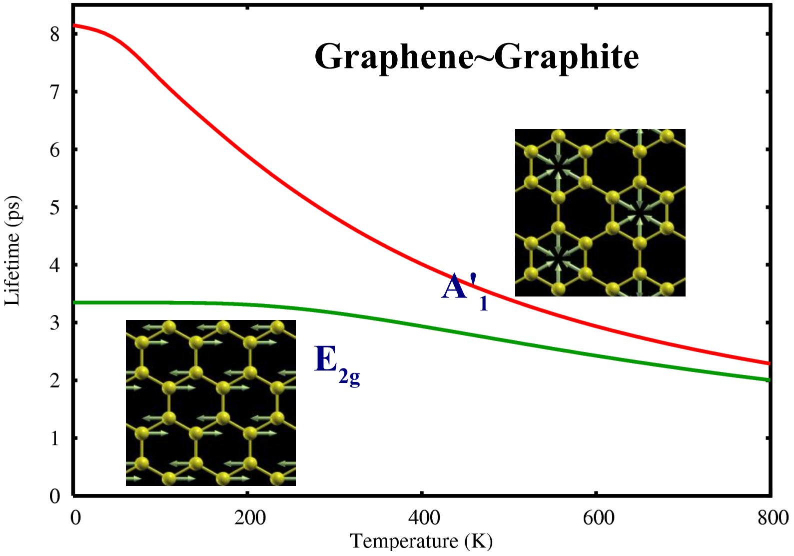
[Bonini, Lazzeri, Marzari, Mauri, Phys. Rev. Lett. 99, 176802 (2007)]

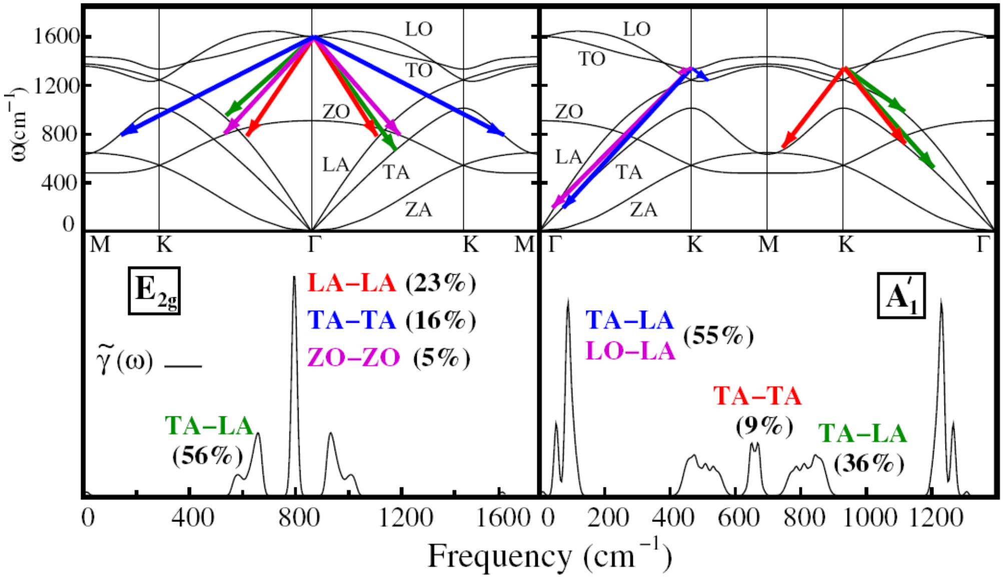


phonon

phonon

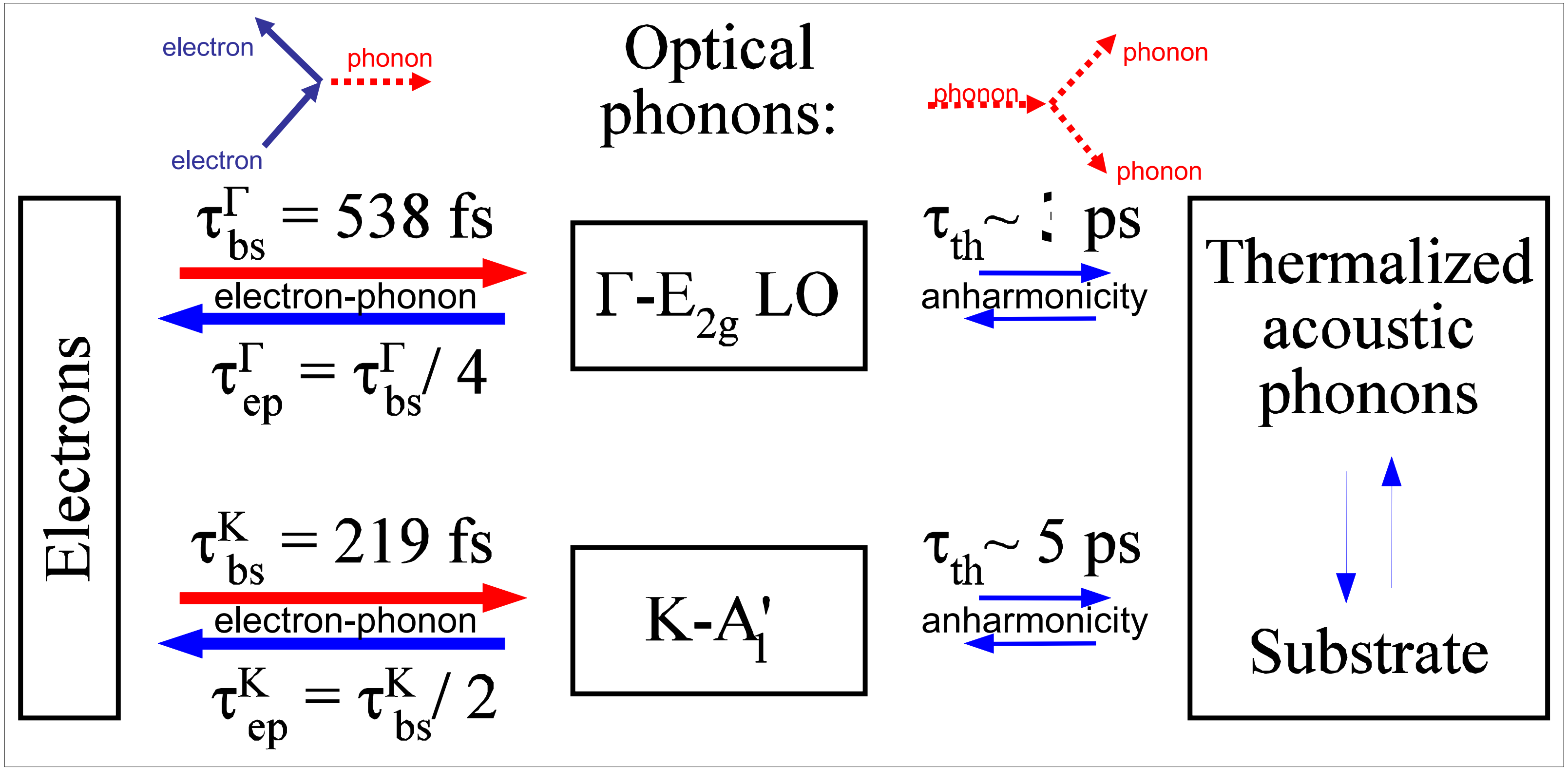
phonon





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



electron

electron

phonon

Optical phonons:

phonon

phonon

phonon

Electrons

$\tau^{\Gamma}_{bs} = 538$ fs

electron-phonon

$\tau^{\Gamma}_{ep} = \tau^{\Gamma}_{bs} / 4$

Γ-E_{2g} LO

$\tau_{th} \sim 3$ ps

anharmonicity

$\tau^{K}_{bs} = 219$ fs

electron-phonon

$\tau^{K}_{ep} = \tau^{K}_{bs} / 2$

K-A_1'

$\tau_{th} \sim 5$ ps

anharmonicity

Thermalized acoustic phonons

Substrate

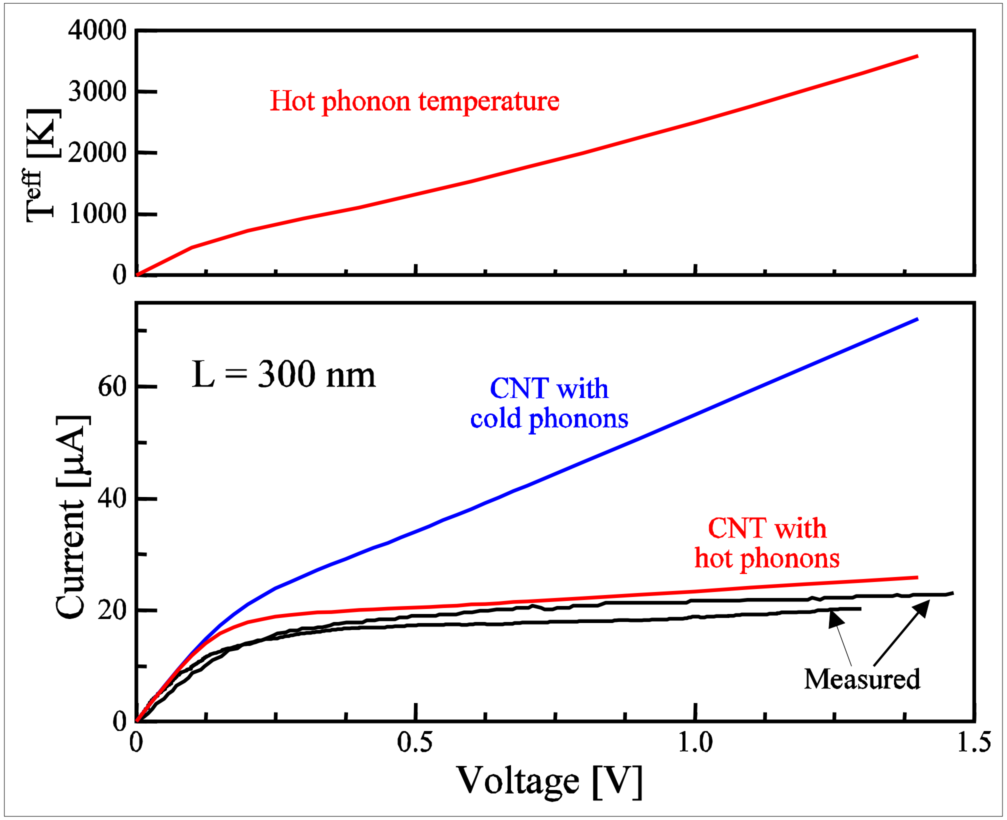
- bottleneck: relaxation from optical to acoustic phonon
- heating of optical phonons is expected

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

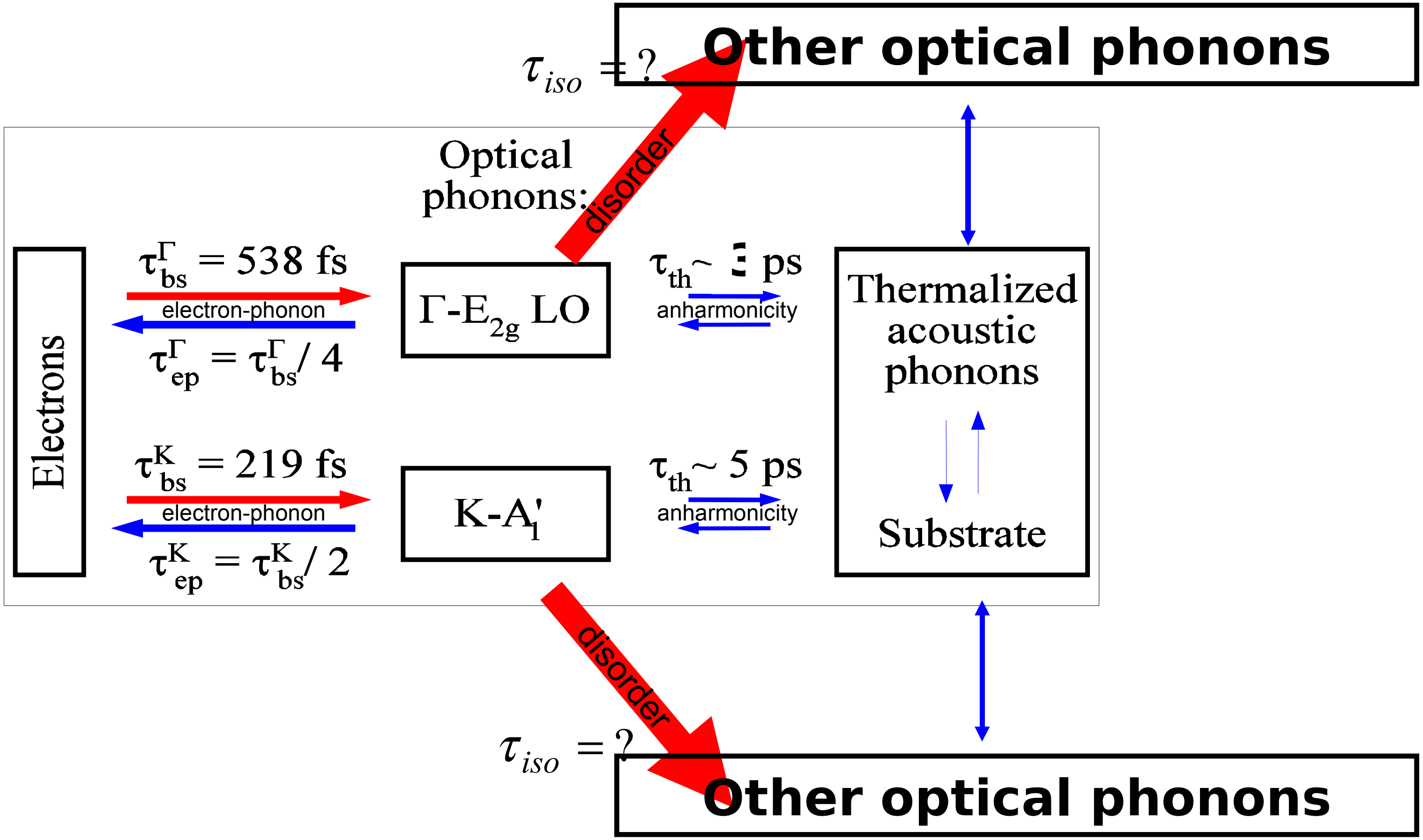
results (300 nm long nanotube)



- 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)]

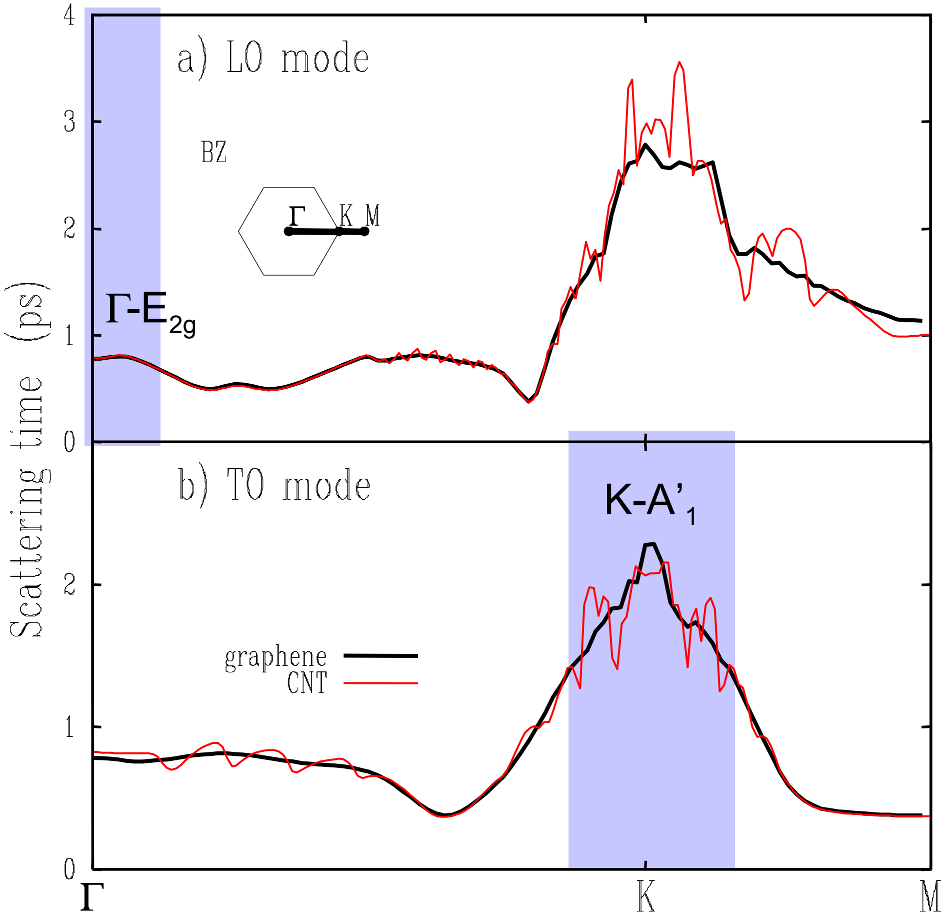


- isotopic disorder scatters phonons but not electrons
- is the disorder-decay-time shorter than τ_{th} (3-5 ps)?

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

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

with x=0.5



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

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

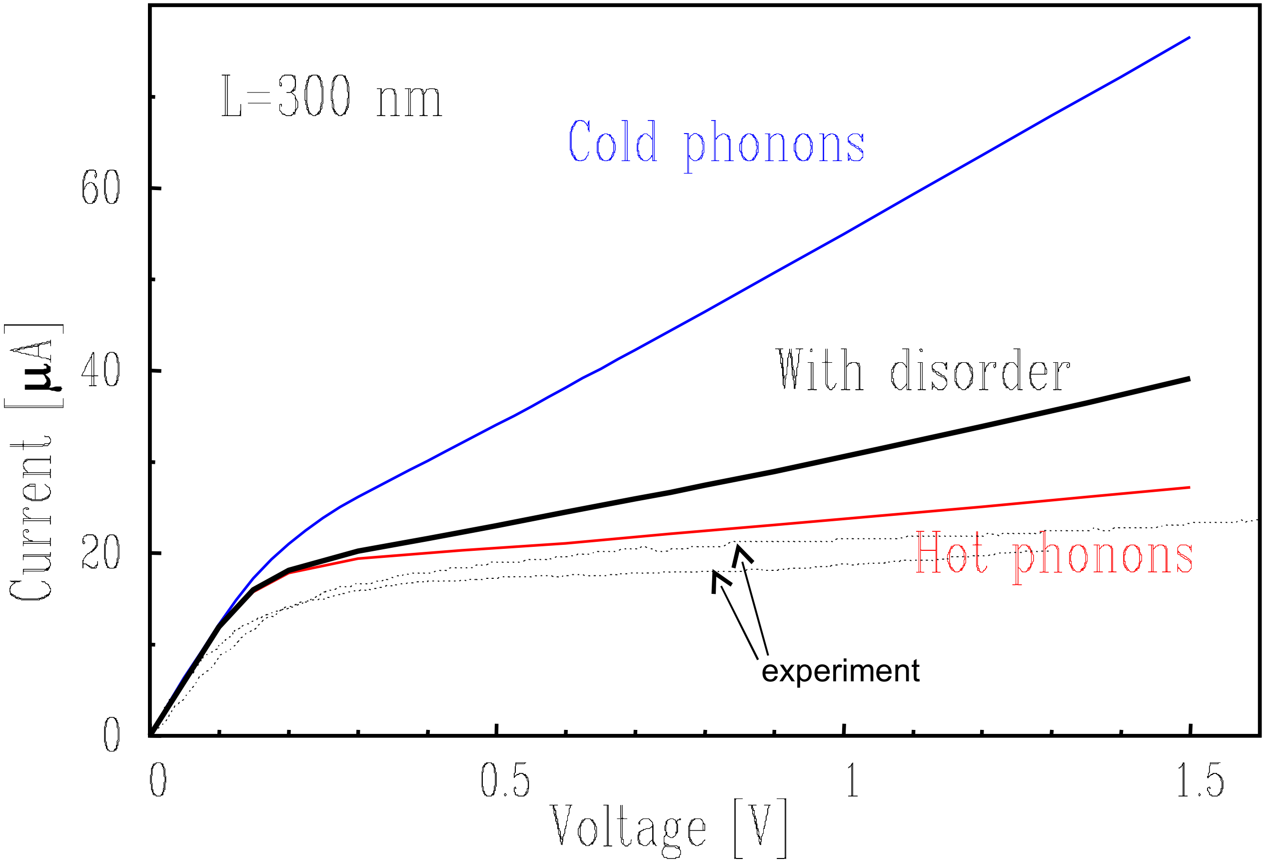
- is the disorder-decay-time shorter than τ_{th} (3-5 ps)?

yes

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

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

with x=0.5



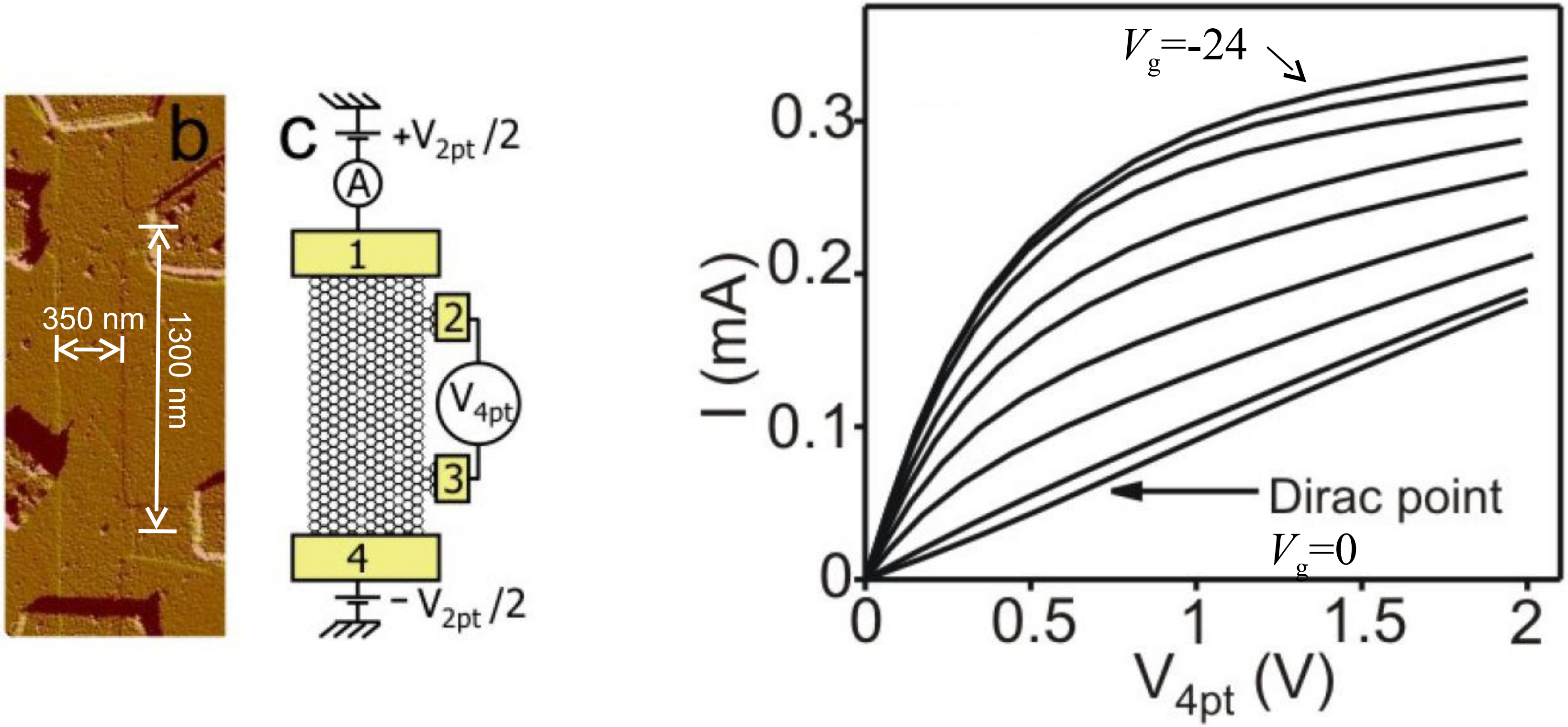
- improvement in the performances (decrease of differential resistivity)

PART 2

GRAPHENE

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

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

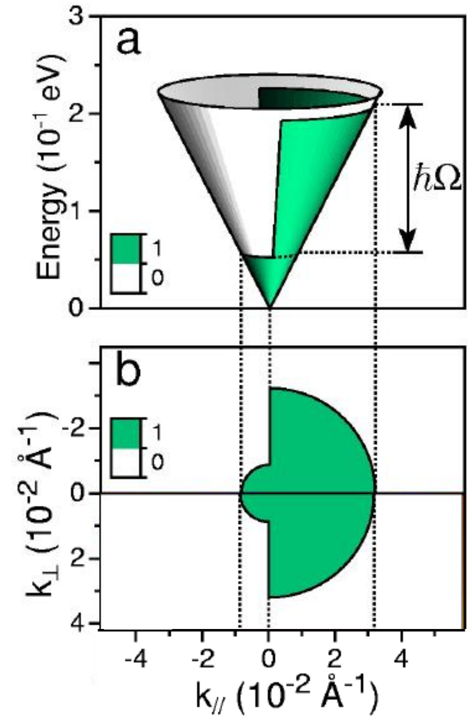


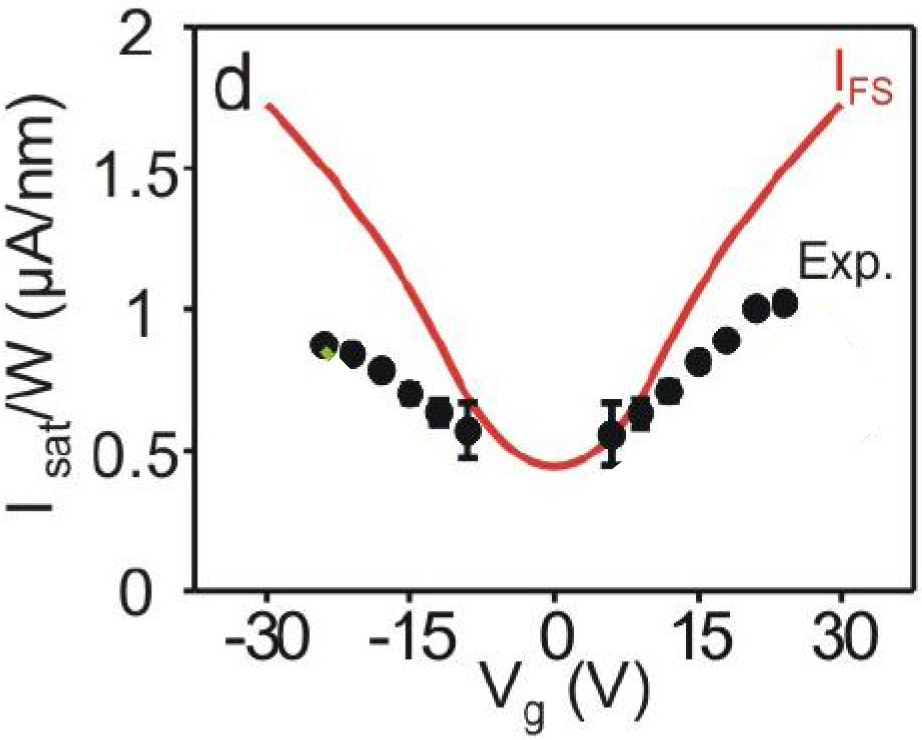
- differential resistance increases by current never fully saturates
- current 350μA/350nm ~ 1 μA/nm. In nanotubes 20μA/(π 2nm) ~ 3μA/nm
- we define a pseudo-sat current, I_{sat}, as the current when $dI/dV=1/(14k\Omega)$

graphene at high bias

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

full saturation model



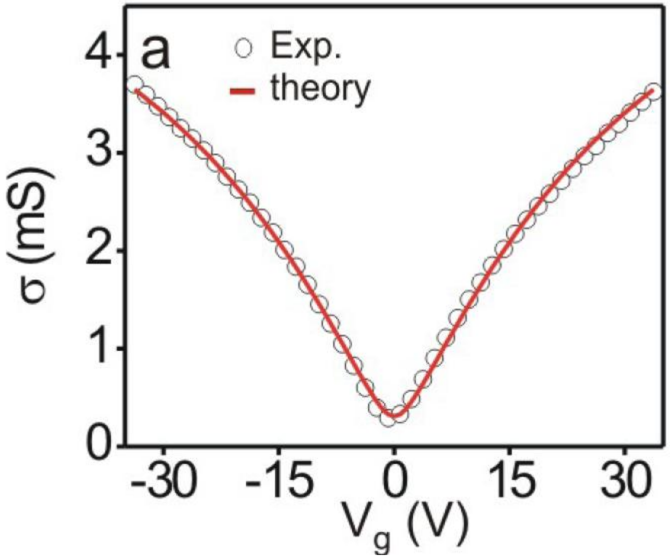


- if phonon emission instantaneous once the threshold is reached and elastic scattering negligible
- this model overestimates the current in graphene

Boltzmann theory for electrons and phonons

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

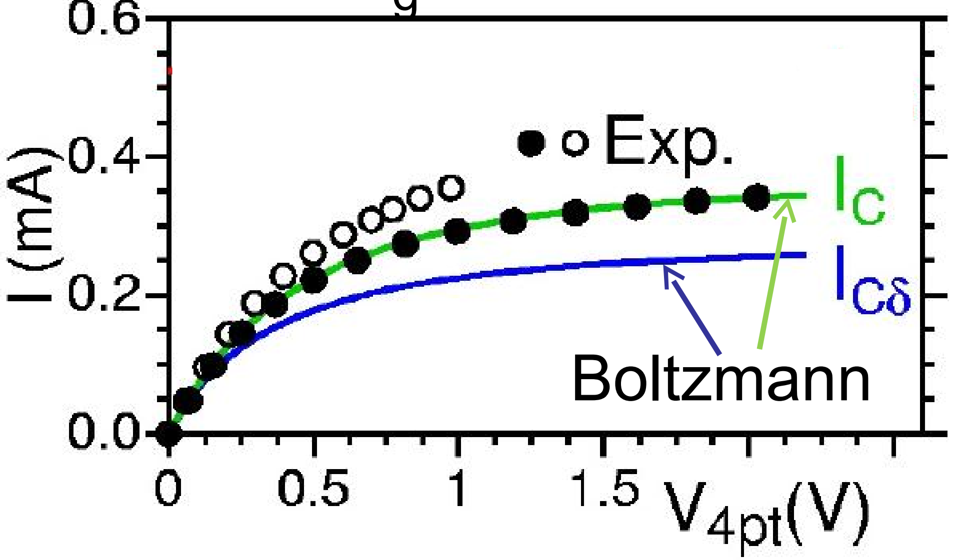
- intrinsic parameters: electron-phonon and phonon-phonon (anharmonic) scattering length from DFT (and GW) calculations validated on experimental phonon measurements.
- extrinsic parameters: elastic scattering length modeled as in [Hwang, Das Sarma, PRB 77, 195412 (2008)]. Free parameters (density of charged and neutral defects) fitted to reproduce the low-bias experimental conductivity. Two models (C and Cδ) equally good at low bias.



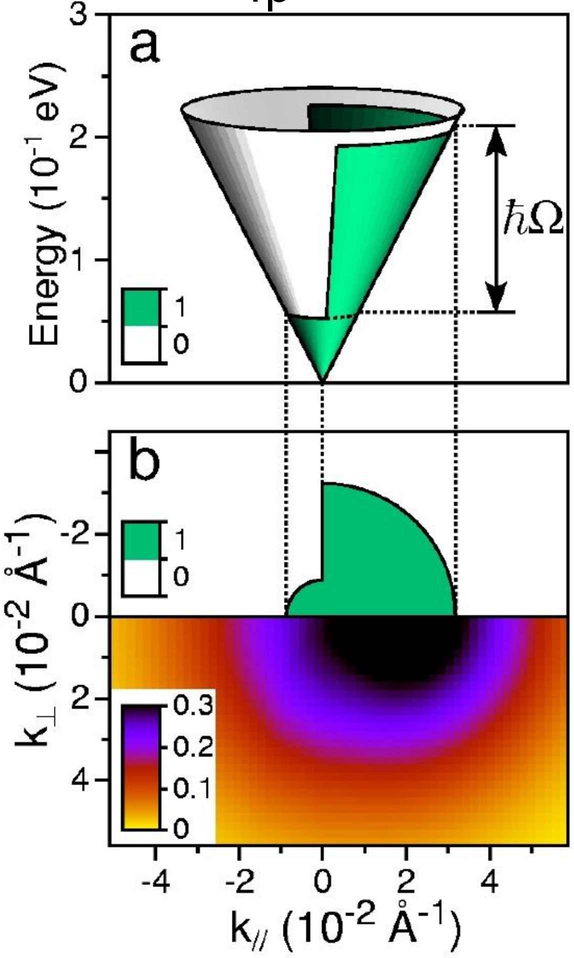
Boltzmann theory for electrons and phonons

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

V_g=+-24V



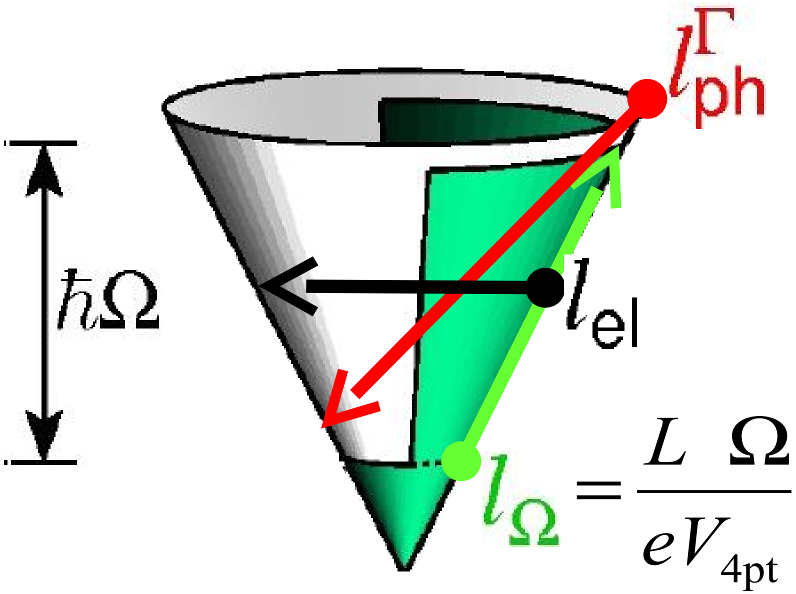
V_{4p}=2V



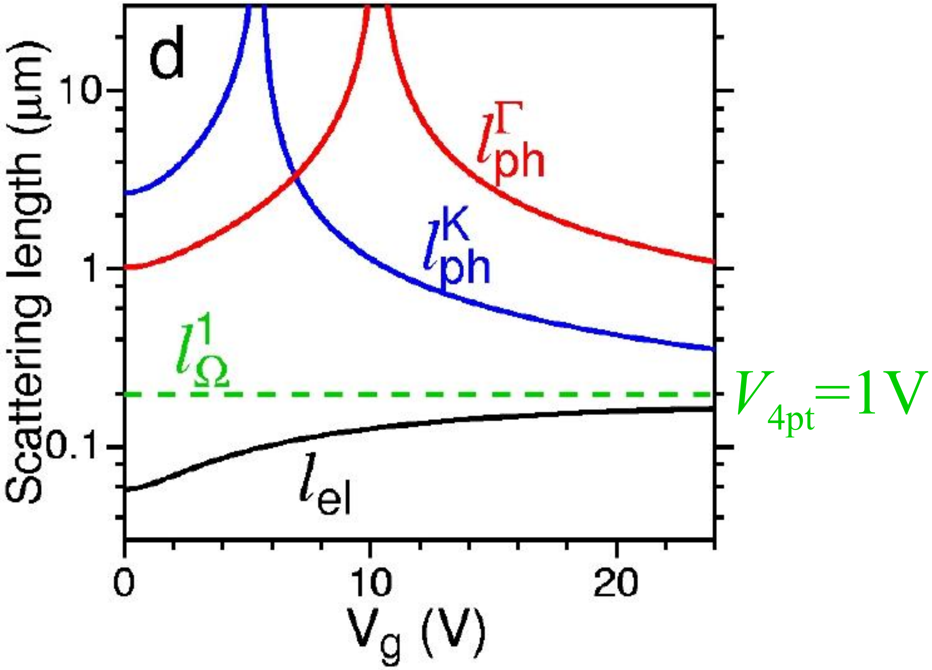
- •Boltzmann reproduces partial saturation seen in expt.
- •phonon remain cold (no hot phonon as in tubes)
- •electron distribution different from full saturation

Scattering lengths in graphene

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



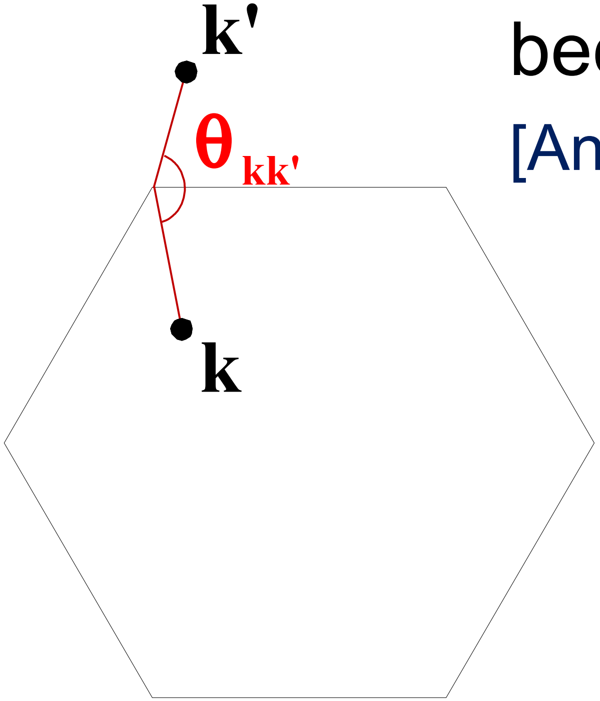
$$l_\Omega = \frac{L\ \ \Omega}{eV_{4pt}}$$



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

- saturation is complete if the phonon emission is instantaneous, $l_\Omega \gg l_{ph}$, and the elastic scattering is negligible, $l_{el} \gg l_\Omega$.

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



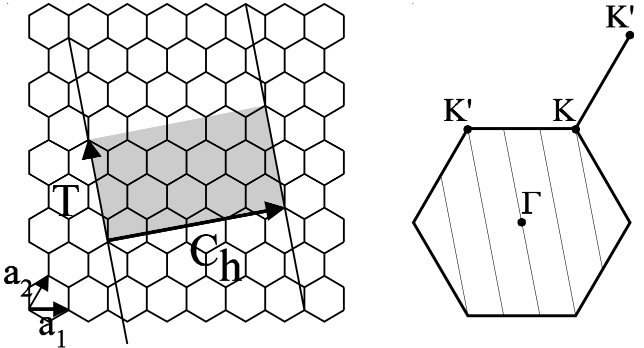
because of pseudospin conservation

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

$$\text{scattering} \propto |V(\mathbf{k}-\mathbf{k}')|^2 \cos^2(\theta_{\mathbf{kk}'}/2)$$

$$= 0 \quad \text{if} \quad \theta_{\mathbf{kk}'} = \pi$$

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



Conclusions

metallic carbon nanotubes

- full saturation is possible, since l_{el} ~ 1000 nm >> l_{ph} ~ 100 nm
- at high bias, since $\tau_{\mathrm{epc}} \ll \tau_{\mathrm{anharmonic}}$, 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
- no hot phonons since $\tau_{\mathrm{epc}} > \tau_{\mathrm{anharmonic}}$
- current per lateral length 1μA/nm
- higher currents are possible by reducing l_{el} or by increasing V_{g}

Anharmonic vs. expt.