Computation with Phonons/Heat

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Centre for Computational Science and Engineering
Department of Physics

Focus Meeting: ***Entropy Production, Transport, Chaos and Turbulence,***
IHP, Paris 5-9 Nov 2007

Outline

Part I: Heat conduction in single walled nanotubes:

Simulation and Experiment

Part II: Computation with Phonons

2.1	Thermal diode/rectifier: rectification of heat flux Simulation and Experiment
2.2	Thermal Transistor: heat switch and modulator
2.3	Thermal logic gates

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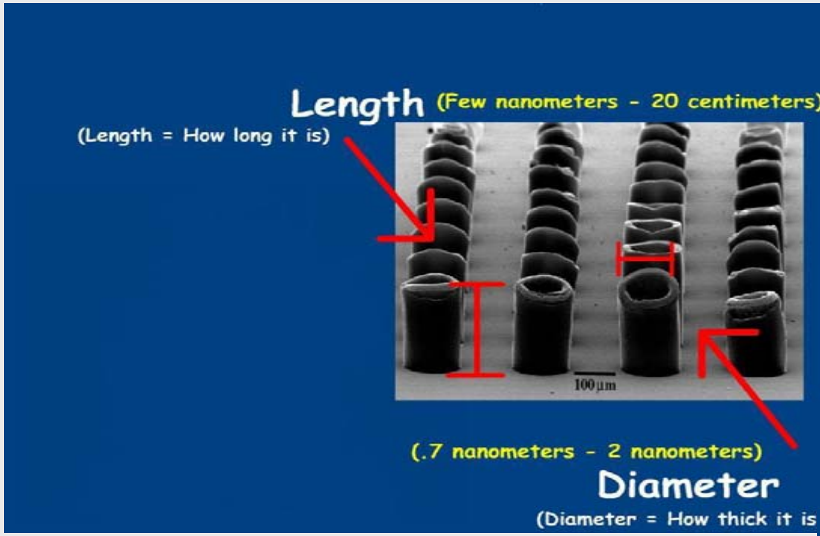
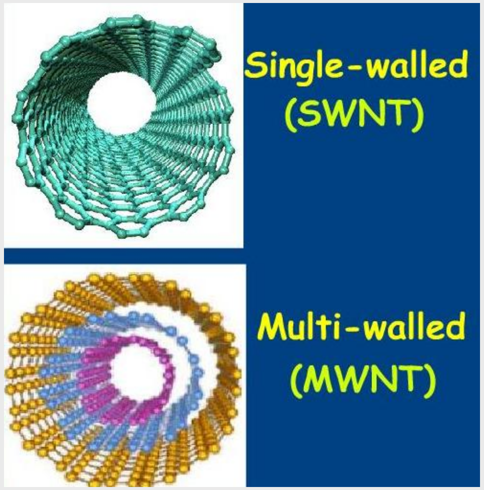
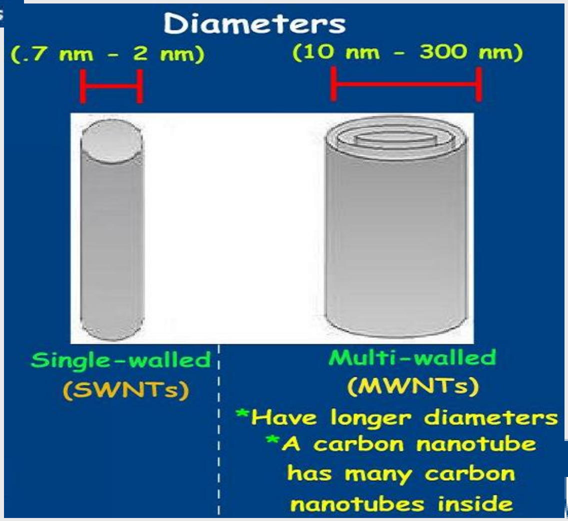
Carbon nanotubes are discovered by Sumio Iijima at NEC labs in 1991.

["Helical microtubules of graphitic carbon", S. Iijima, Nature 354**, 56 (1991)]**



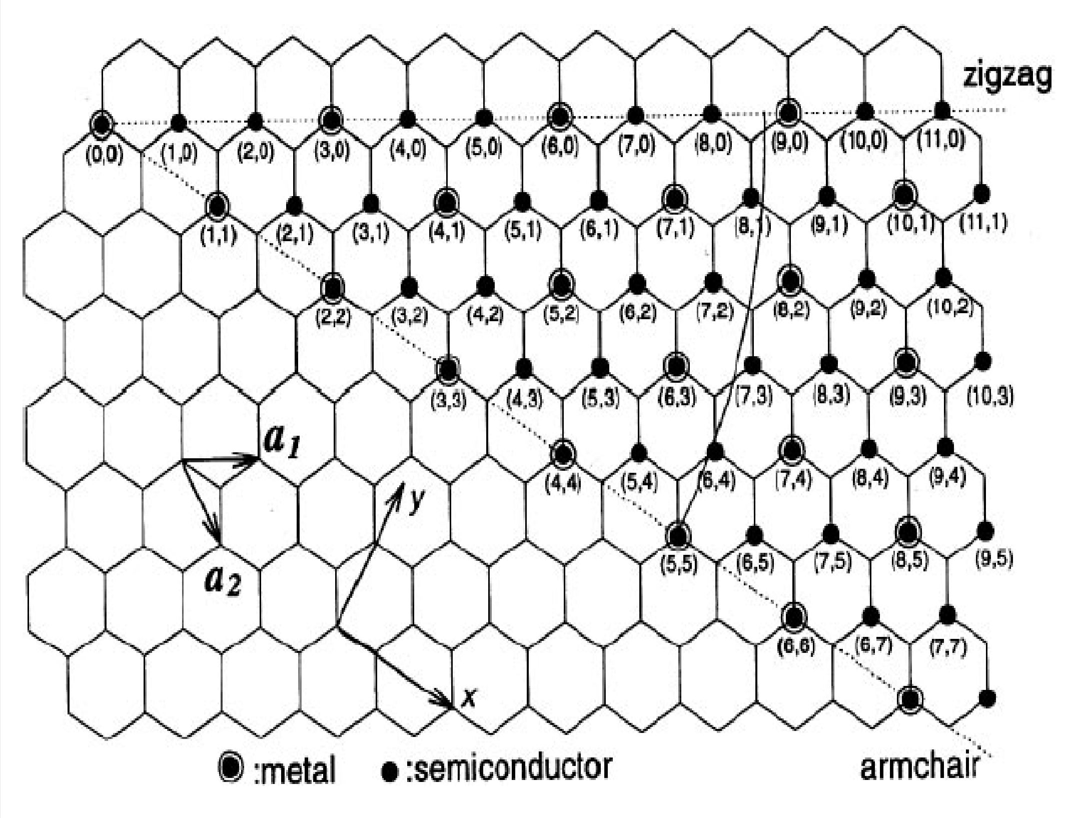


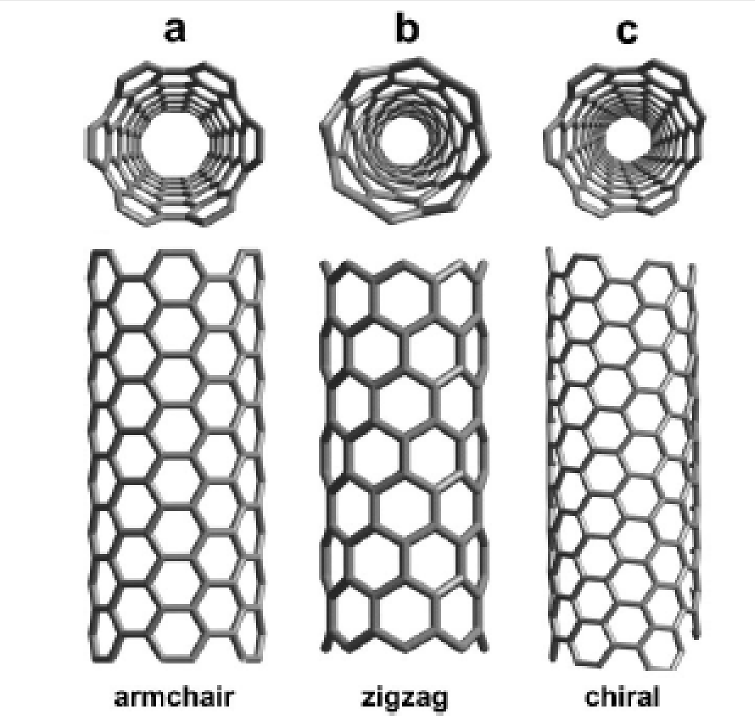


*Have longer diameters

*A carbon nanotube has many carbon nanotubes inside

Types of single walled nanotubes



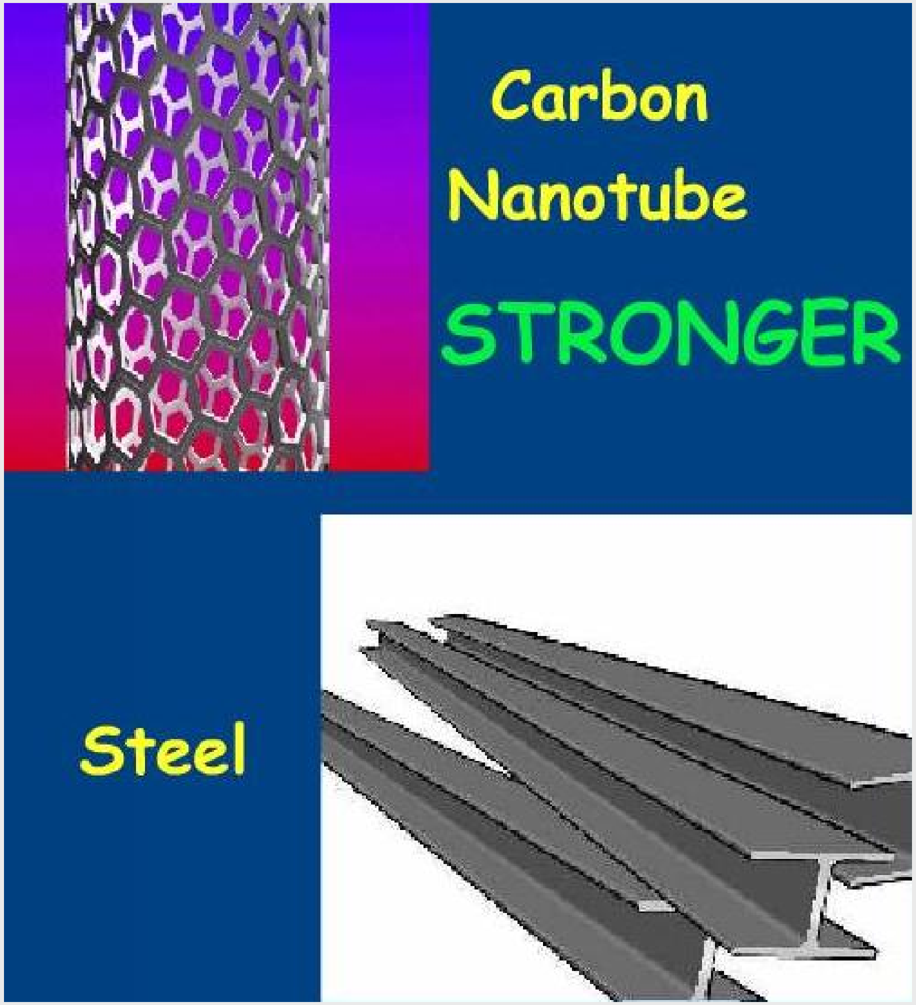


- **The tubes of indices (*m, n*) with (*m - n*) a multiple of *3* are metallic. The rest will be semiconductors.**

They are *100* times stronger than steel,

but weight

only *one-sixth* as much!

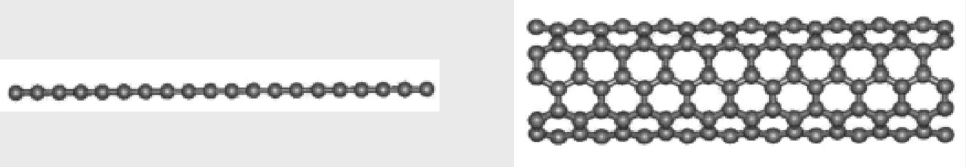


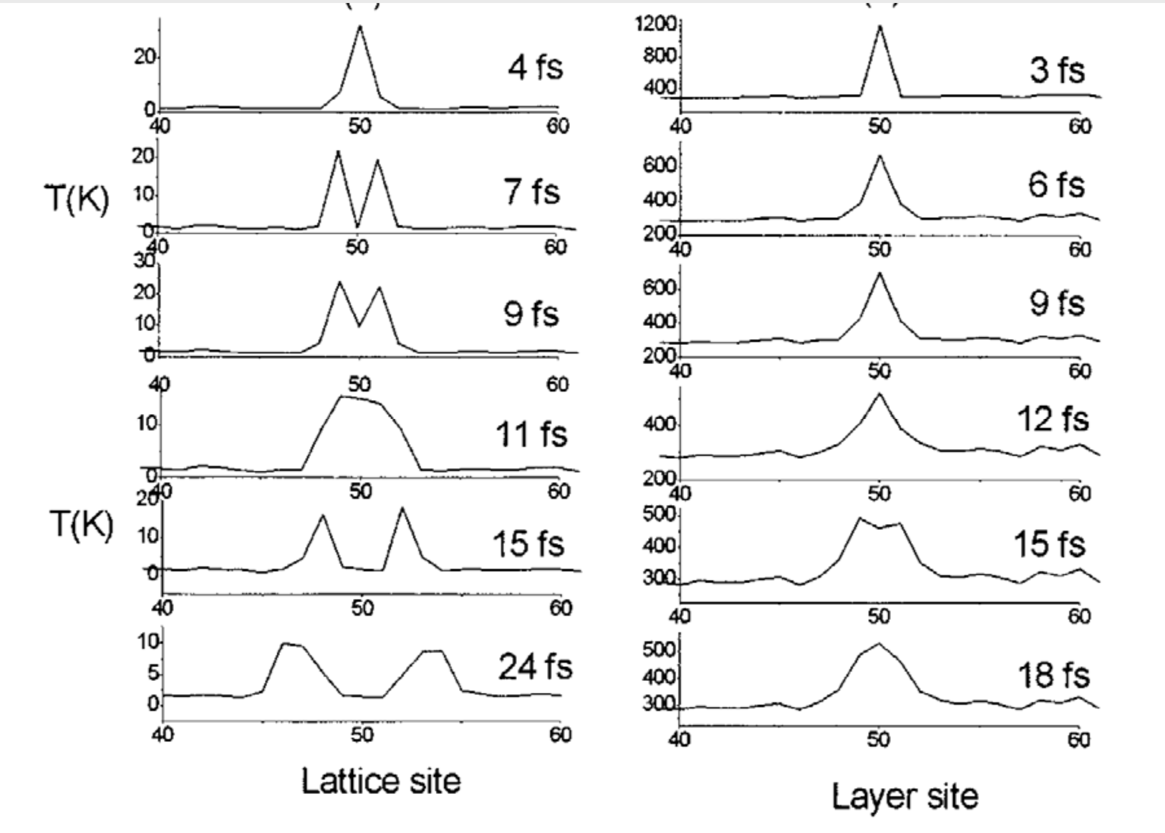
Thermal conductivity?

- **How is vibrational energy transported?**
- **Whether Fourier law is still valid for heat conduction in nanotube?**
- **Is nanotube a one dimensional conductor or a quasi-1d conductor?**
- **How does temperature, tube radius, isotop impurity, and chirality affect thermal conductivity?**

Anomalous diffusion in nanotubes

G Zang and BL, J. Chem. Phys. 123, 014705 (2005)





Anomalous diffusion in nanotubes

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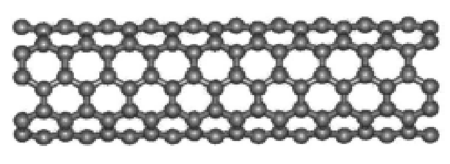


Fig.2

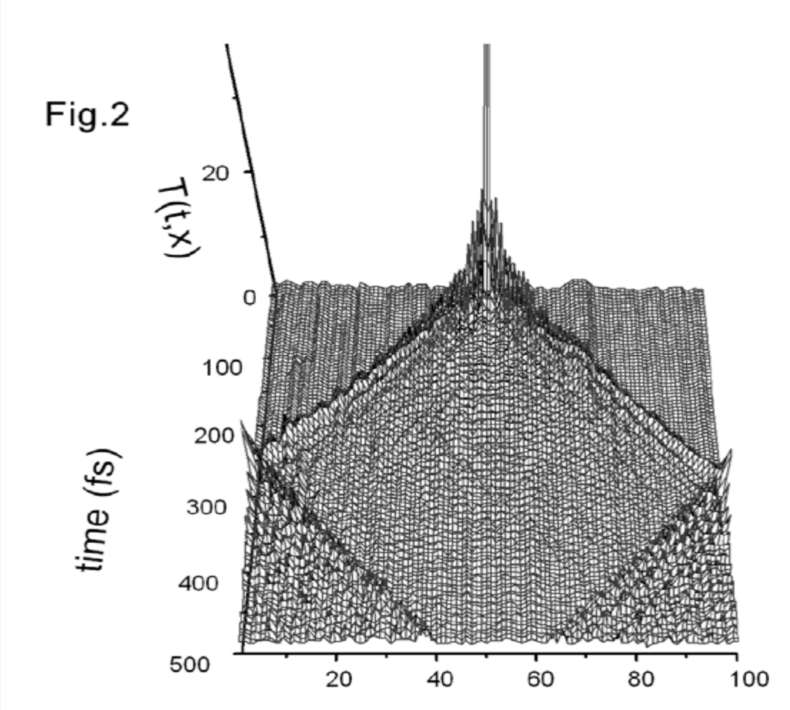
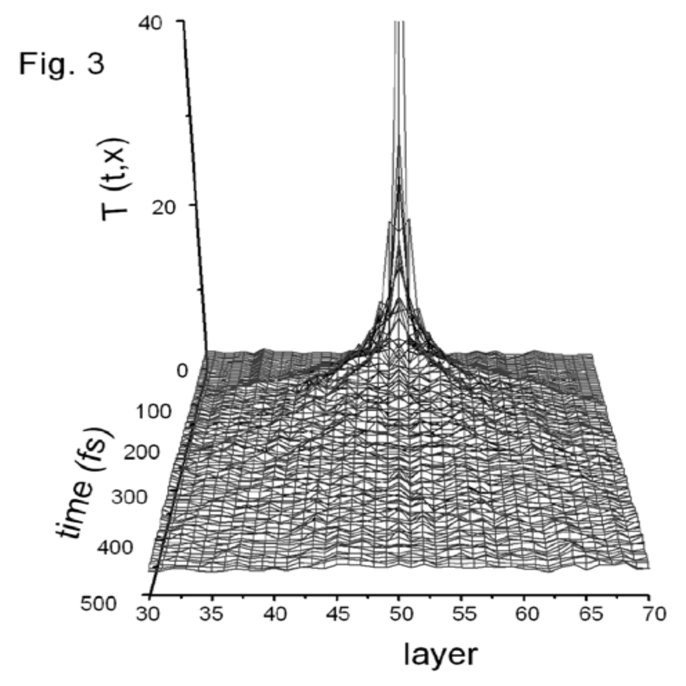


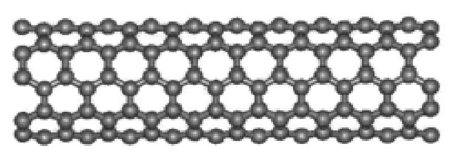
Fig. 3

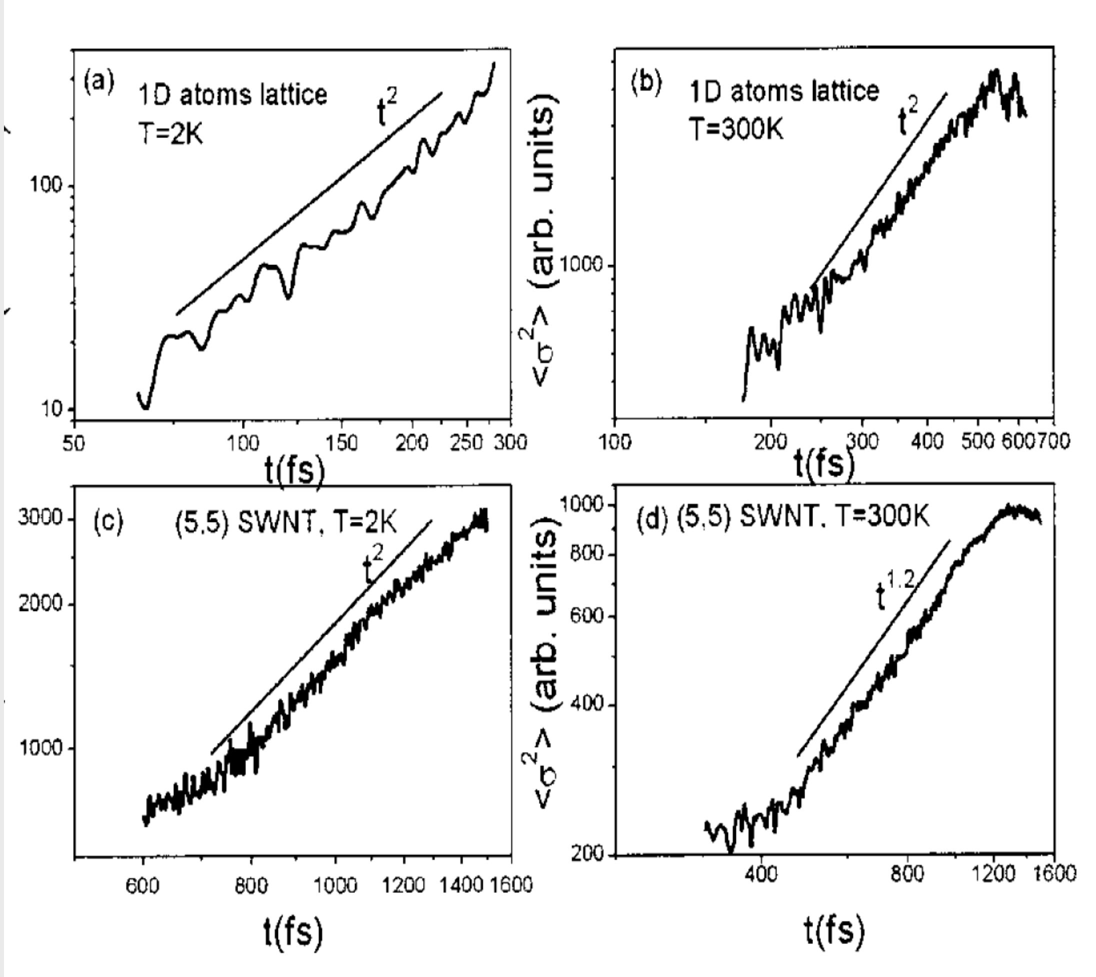


Anomalous diffusion in nanotubes

G Zang and BL, J. Chem. Phys. 123, 014705 (2005)

$$\sigma^2(t) = \frac{\int (E(x,t) - E_0)(x - x_0)^2 dx}{\int (E(x,t) - E_0) dx},$$





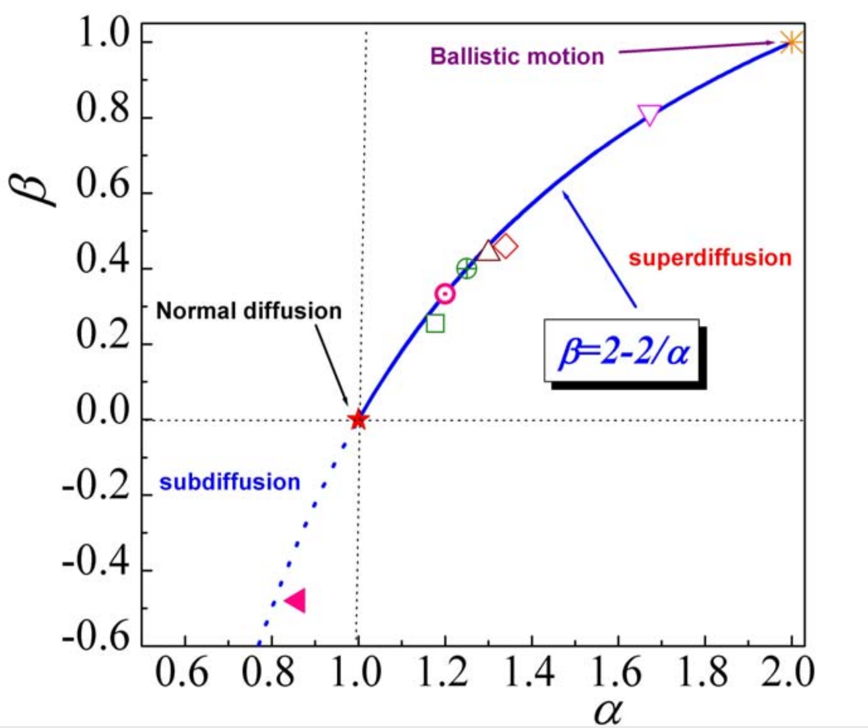
Anomalous heat conduction and anomalous diffusion

BL and J Wang, PRL 91, 044301 (2003)

$$\left\langle (\Delta x)^2 \right\rangle = 2Dt^{\alpha}$$

$$\kappa = -J/(dT/dx) \sim L^{\beta}$$

$$\beta = 2 - 2/\alpha$$



$$\left.\begin{array}{l} \alpha < 1: \text{Subdiffusion} \\ \alpha = 1: \text{Normal diffusion} \\ \alpha > 1: \text{Superdiffusion} \\ \alpha = 2: \text{Ballistic motion} \end{array}\right\} \Longleftrightarrow \left\{\begin{array}{l} \beta < 0, \text{ Convergent } \kappa. \\ \beta = 0, \text{ Fourier law } \kappa = \text{Const.} \\ 0 < \beta < 1, \text{ Divergent } \kappa. \\ \beta = 1, \kappa \propto \text{L}. \end{array}\right.$$

For nanotube $\alpha = 1.2 \longrightarrow \beta = 0.33$

Length dependent thermal conductivity of SWCN

S Maruyama, Physica B. 323, 193 (2002)

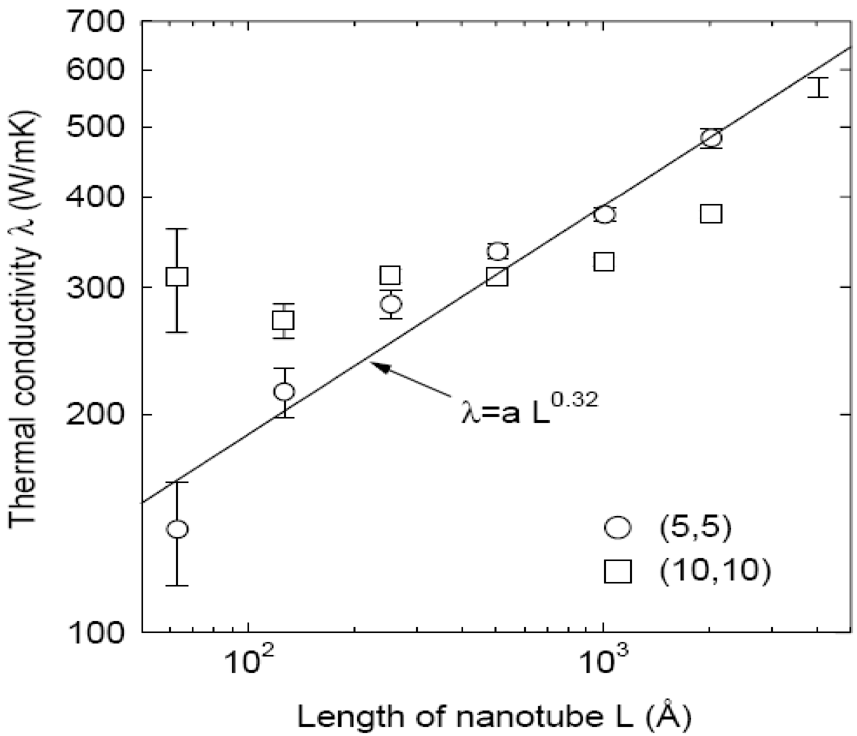
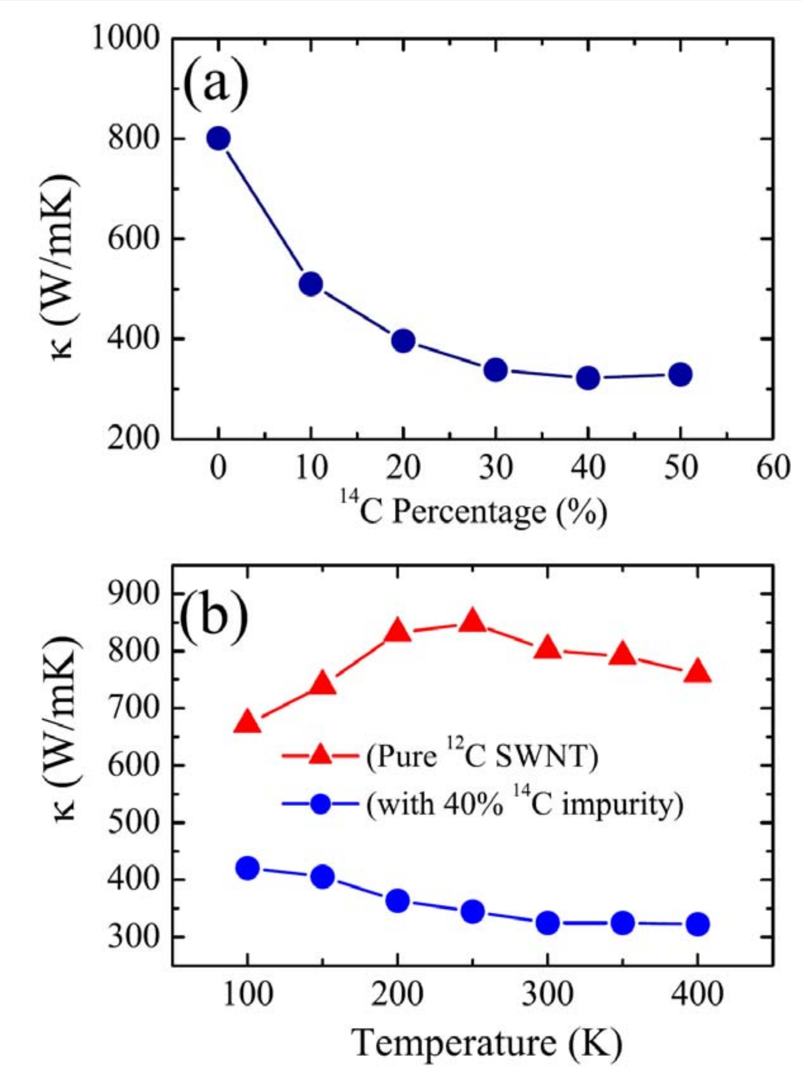


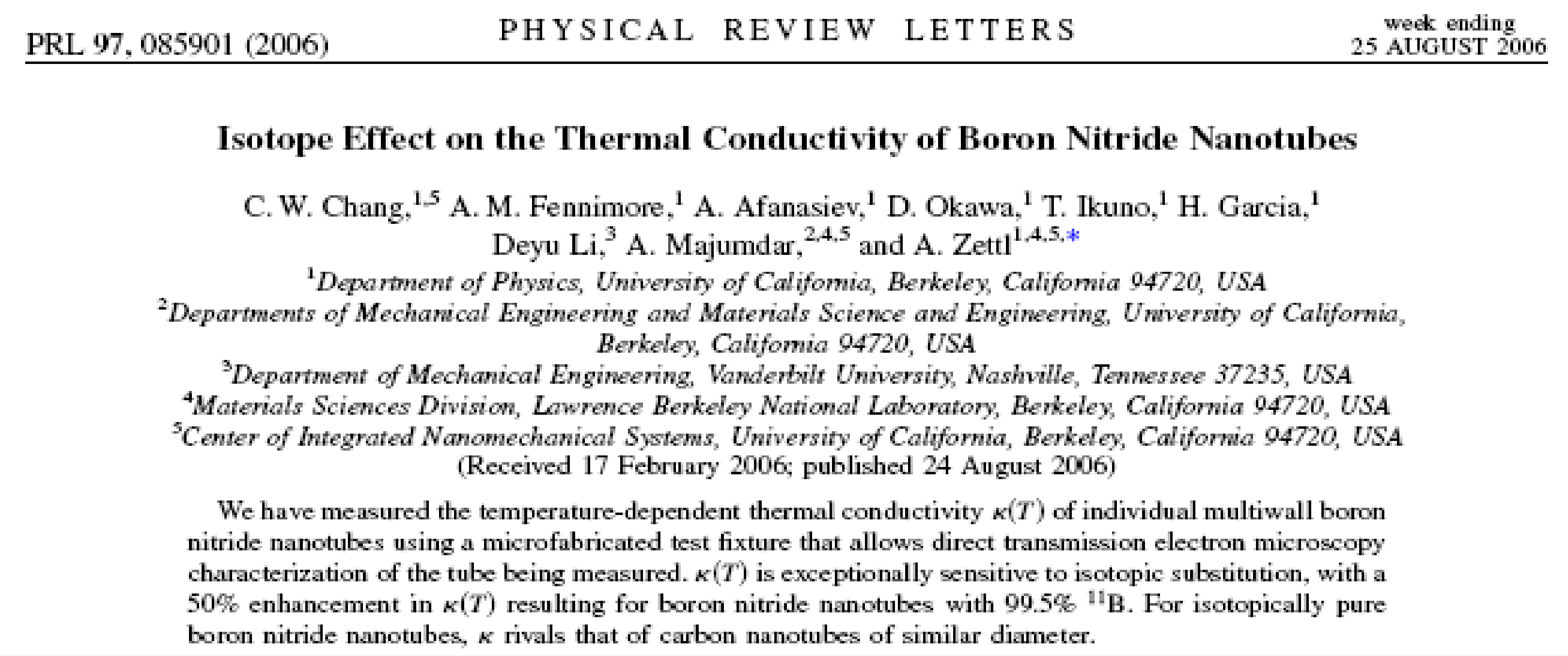
Fig. 1. Dependence of thermal conductivity on length of nanotubes for 300 K.

Heat conductivity: Effects of isotope

G Zang and BL, J. Chem. Phys. 123, 114714 (2005)



Experiment confirmation



PRL 97, 085901 (2006) PHYSICAL REVIEW LETTERS week ending 25 AUGUST 2006

Isotope Effect on the Thermal Conductivity of Boron Nitride Nanotubes

C. W. Chang,[1,5] A. M. Fennimore,[1] A. Afanasiev,[1] D. Okawa,[1] T. Ikuno,[1] H. Garcia,[1]
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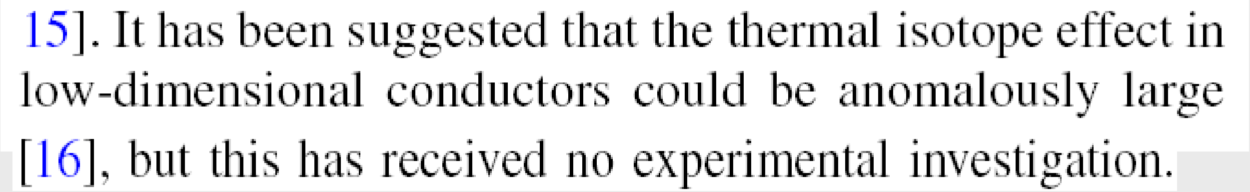
(Received 17 February 2006; published 24 August 2006)

We have measured the temperature-dependent thermal conductivity $\kappa(T)$ of individual multiwall boron nitride nanotubes using a microfabricated test fixture that allows direct transmission electron microscopy characterization of the tube being measured. $\kappa(T)$ is exceptionally sensitive to isotopic substitution, with a 50% enhancement in $\kappa(T)$ resulting for boron nitride nanotubes with 99.5% ^{11}B. For isotopically pure boron nitride nanotubes, κ rivals that of carbon nanotubes of similar diameter.



15]. It has been suggested that the thermal isotope effect in low-dimensional conductors could be anomalously large [16], but this has received no experimental investigation.

[16] G. Zhang and B. W. Li, J. Chem. Phys. **123**, 114714 (2005).

Experimental set up

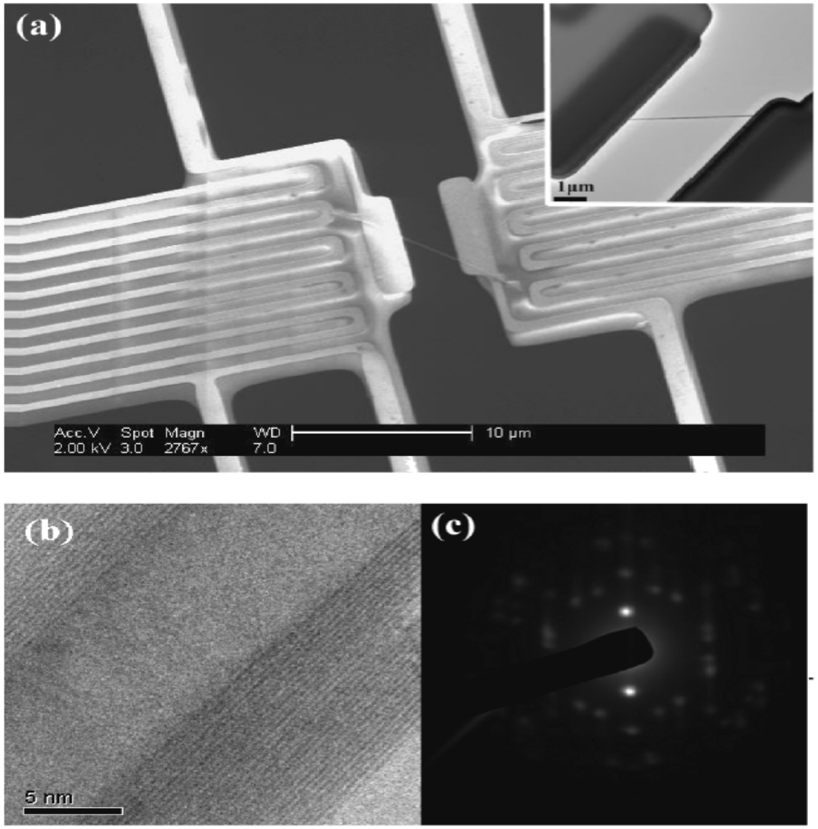


FIG. 1. (a) A scanning electron microscope image of the microfabricated test fixture with a boron nitride nanotube on it (scale bar = 10 μm). The inset shows the corresponding transmission electron microscope image of the same device (scale bar = 1 μm). (b) A high-resolution transmission electron microscope image of the boron nitride nanotube (scale bar = 5 nm). (c) The corresponding electron diffraction pattern of the boron nitride nanotube.

Experimental confirmation

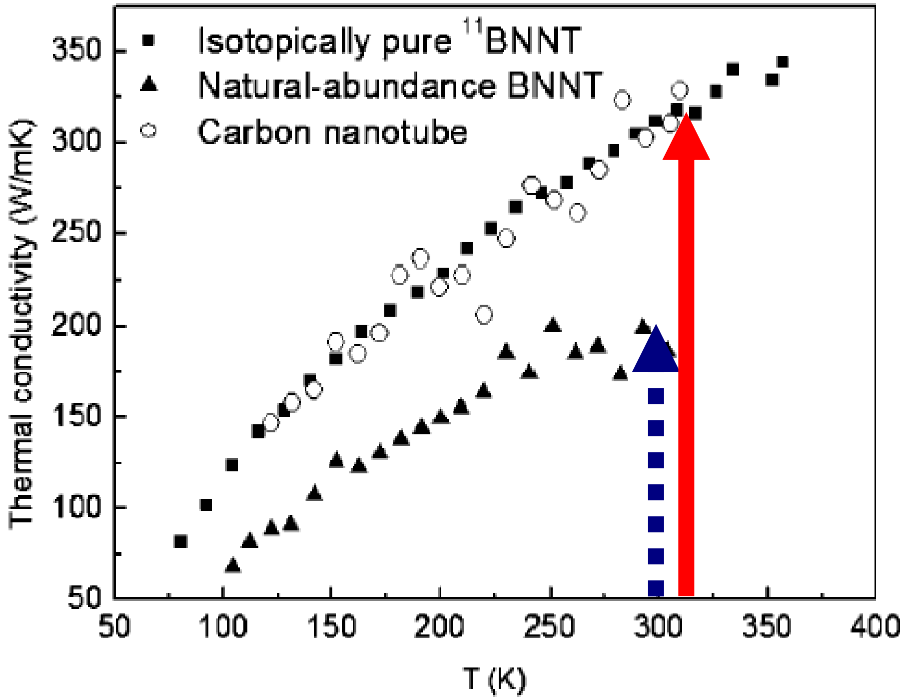
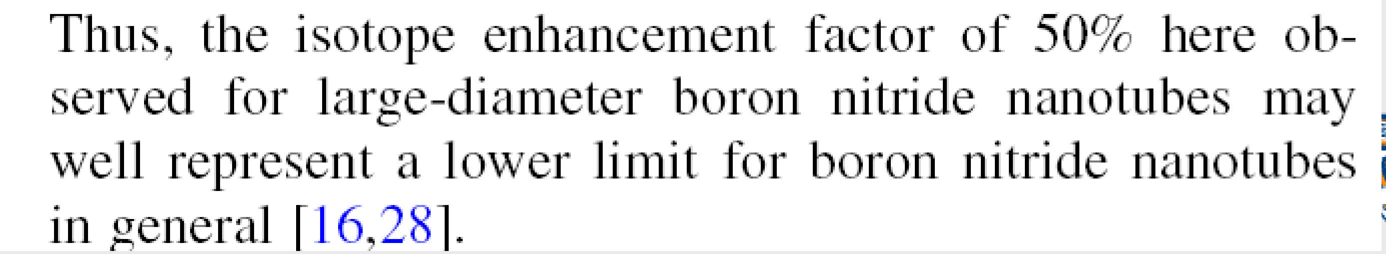


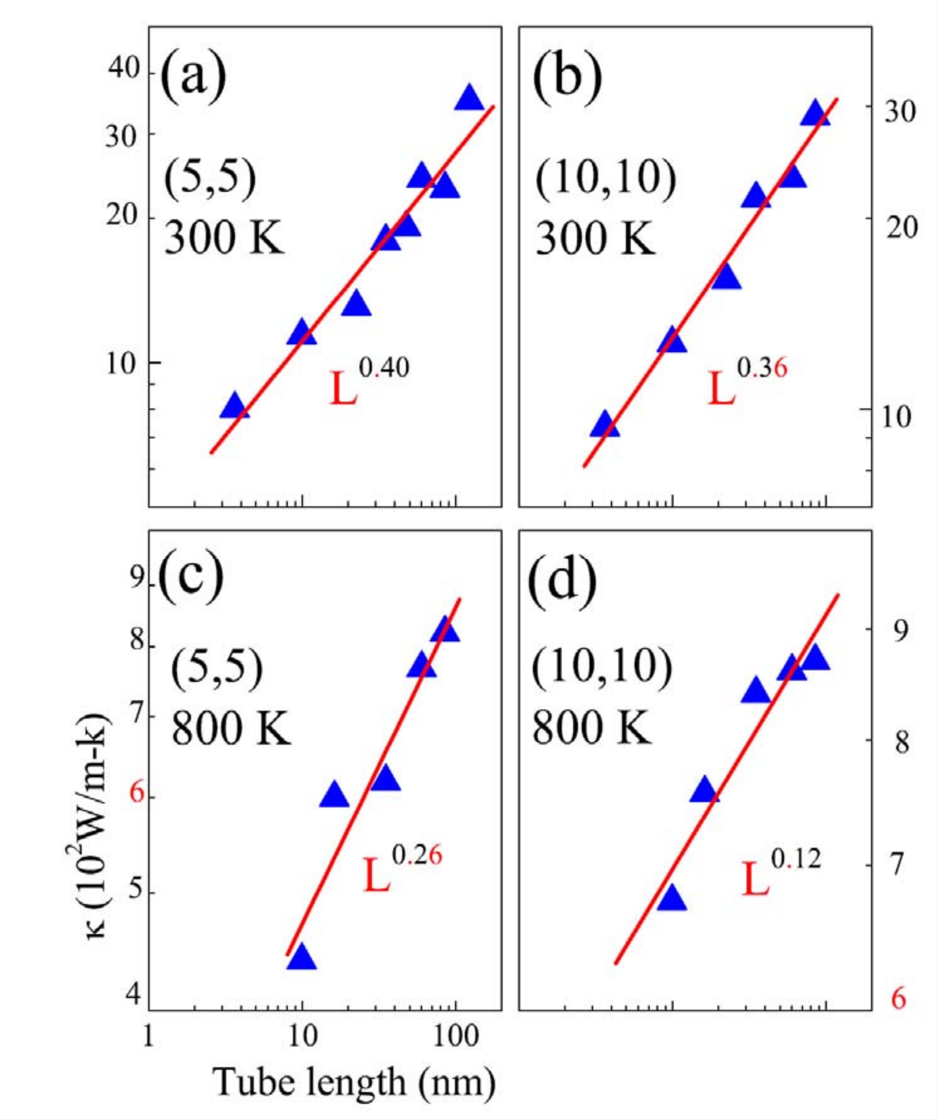
FIG. 2. The $\kappa(T)$ of a carbon nanotube (open circles), a boron nitride nanotube (BNNT, solid triangles), and an isotopically pure boron nitride nanotube (solid squares) with similar outer diameters



Thus, the isotope enhancement factor of 50% here observed for large-diameter boron nitride nanotubes may well represent a lower limit for boron nitride nanotubes in general [16,28].

Heat conductivity: Effects of temperature and radius

G Zang and BL, J. Chem. Phys. 123, 114714 (2005).



Summary of heat conduction in SWCN

- Vibrational energy transports super-difussively.
- Thermal conductivity diverges with the length of nanotube.
- The divergent exponent depends on temperature, tube radius and …
- Isotope impurity can reduce the thermal conductivity as much as 50%. (Confirmed by experiment!)
- Chirality has not much affect on thermal conductivity.

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Diode: one way street of current

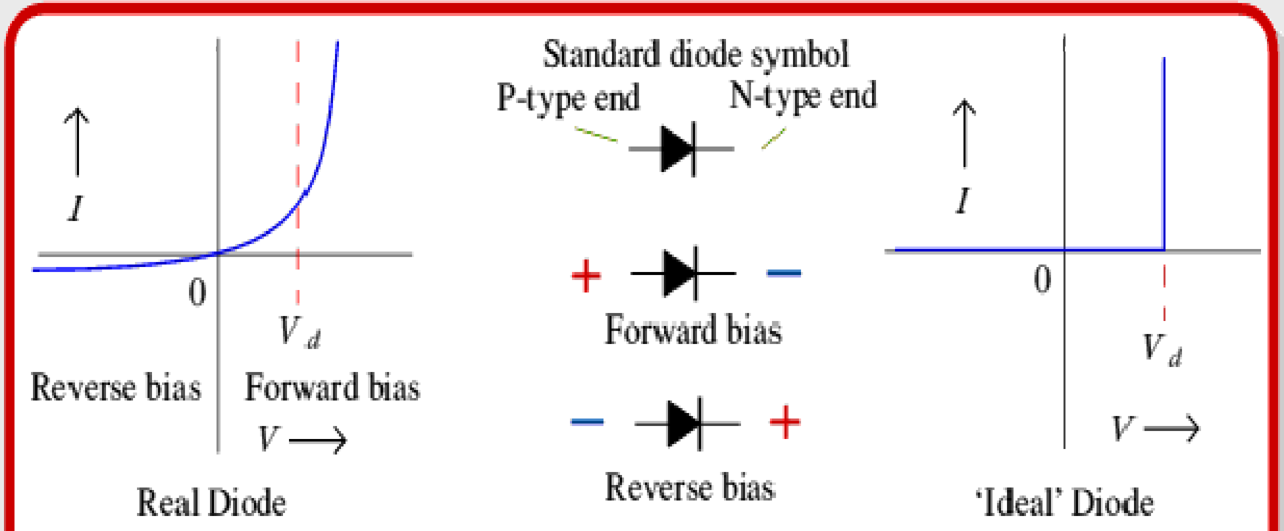


Fig 6.5 Current-Voltage Behaviour of a diode.

Thermal diode/Rectifier

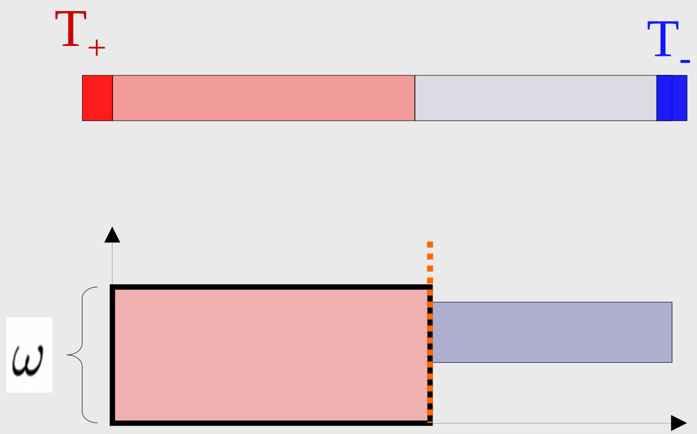
Thermal diode/rectifier

Can we control heat flow in solid state device?

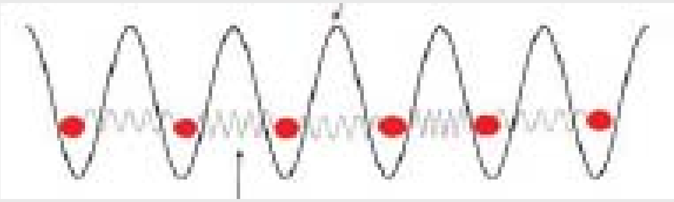
If $T_L > T_R$, heat flows from left to right.

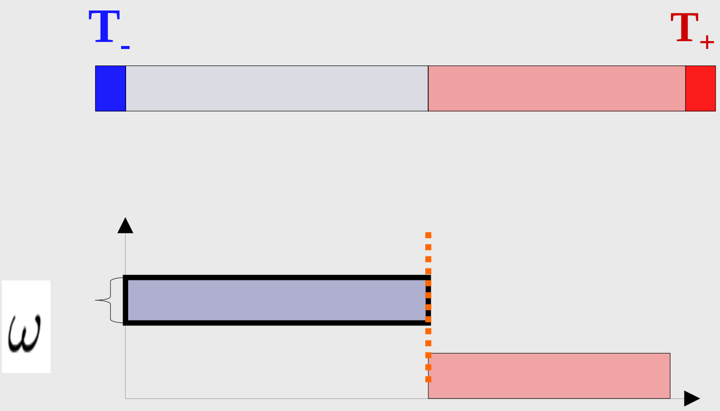
If $T_L < T_{R,}$ heat flow is inhibited from right to left.

Thermal diode: Model I



$$H=\sum\frac{p_i^2}{2m}+\frac{1}{2}k(x_i-x_{i+1}-a)^2-\frac{V}{(2\pi)^2}\cos 2\pi x_i,$$





High temperature limit

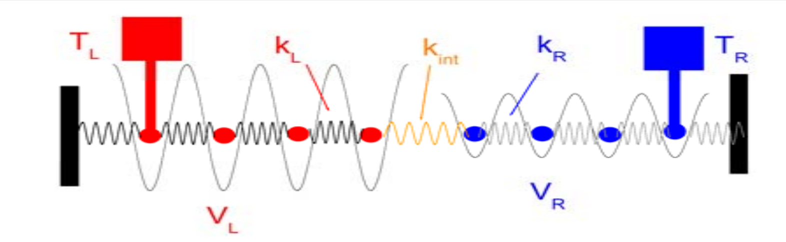
$$0<\omega<2\sqrt{k},$$

Low temperature limit

$$\sqrt{V}<\omega<\sqrt{V+4k}.$$

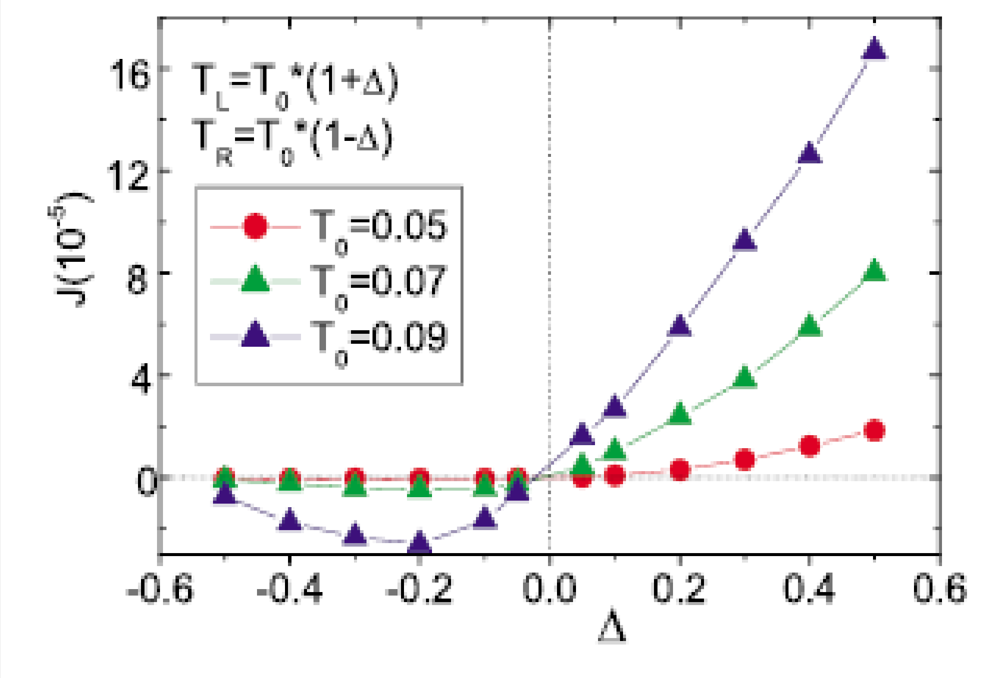
Configuration of the diode model from two coupled nonlinear oscillator chains

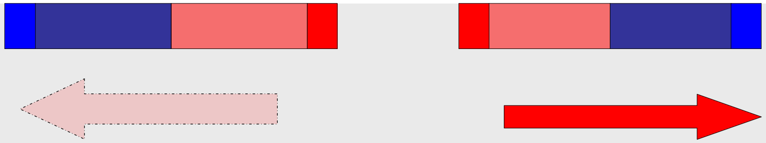
BL, L Wang, and G. Casati, Phys. Rev. Lett. 94, 114101 (2004)



$$k_R = \lambda k_L, \quad V_R = \lambda V_L$$

$$T_L = T_0(1+\Delta), \quad T_R = T_0(1-\Delta)$$





Interface temperature jump

Li et al. Phys. Rev. Lett. 95, 104302 (2005)

Kapitza resistance

$$R \equiv \frac{\Delta T}{J},$$

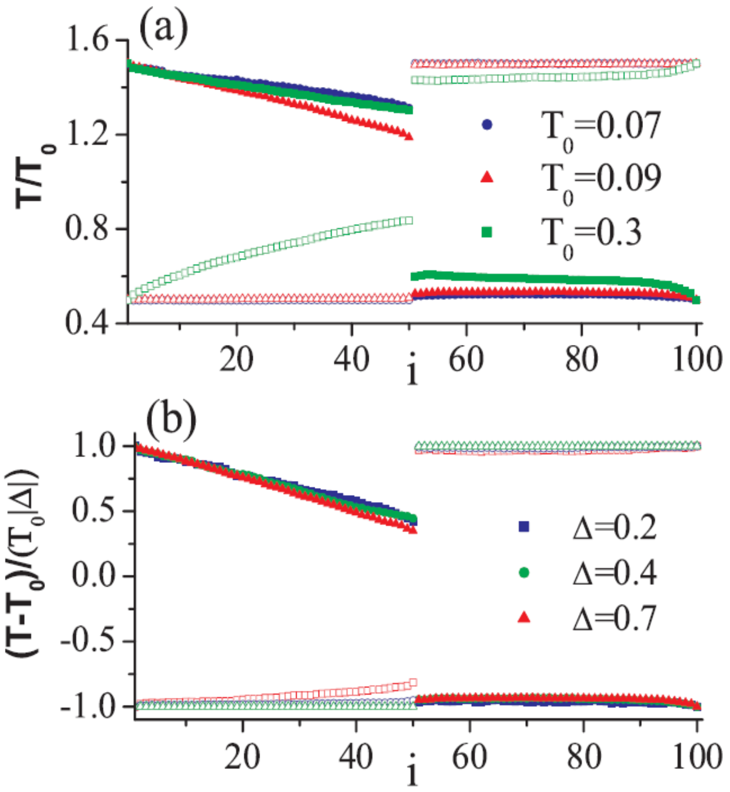


FIG. 2 (color online). (a) T/T_0 versus lattice site for $T_0 =$ 0.07, 0.09, and 0.3. $|\Delta| = 0.5$. (b) $(T - T_0)/(T_0|\Delta|)$ versus lattice site, for different $|\Delta| = 0.2$, 0.4, and 0.7 with fixed $T_0 =$ 0.09. The solid symbols are for the cases of $\Delta > 0$, and the open ones are for the cases of $\Delta < 0$. In both (a) and (b) $N = 50$.

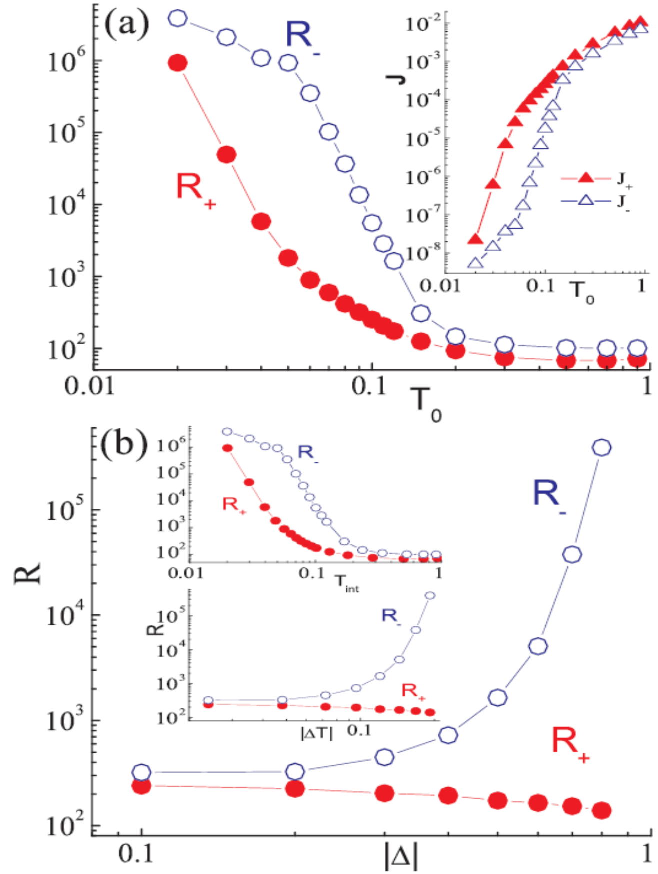
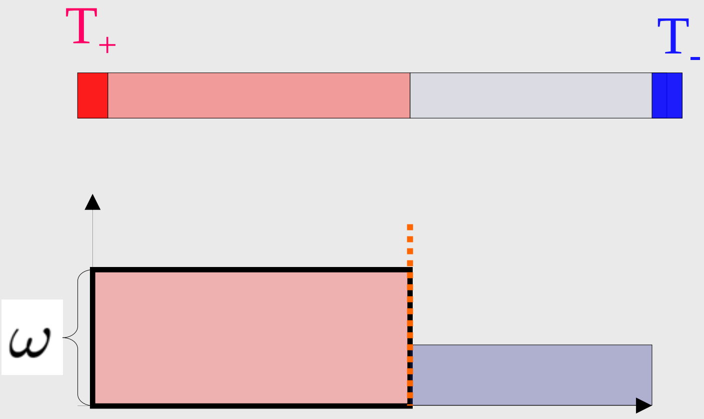
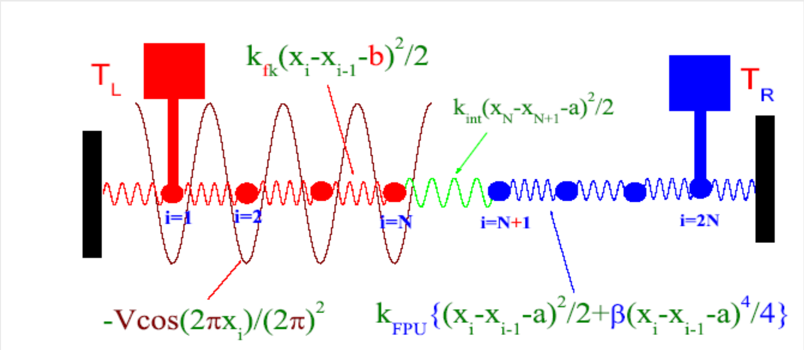


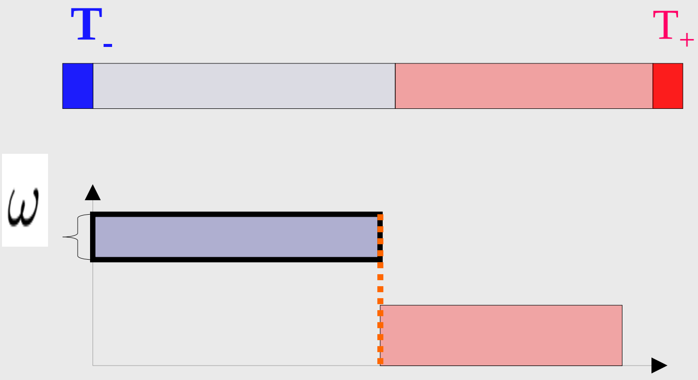
FIG. 3 (color online). (a) $R_\pm$ versus T_0. $|\Delta| = 0.5$. Inset is heat current $J_\pm$ versus T_0. (b) $R_\pm$ versus $|\Delta|$ for $T_0 = 0.12$. Inset of (b) is $R_\pm$ versus interface temperature $T_{\rm int} = (T^L_{\rm int} + T^R_{\rm int})/2$, and $R_\pm$ versus interface temperature jump, ΔT. In all cases $N = 50$.

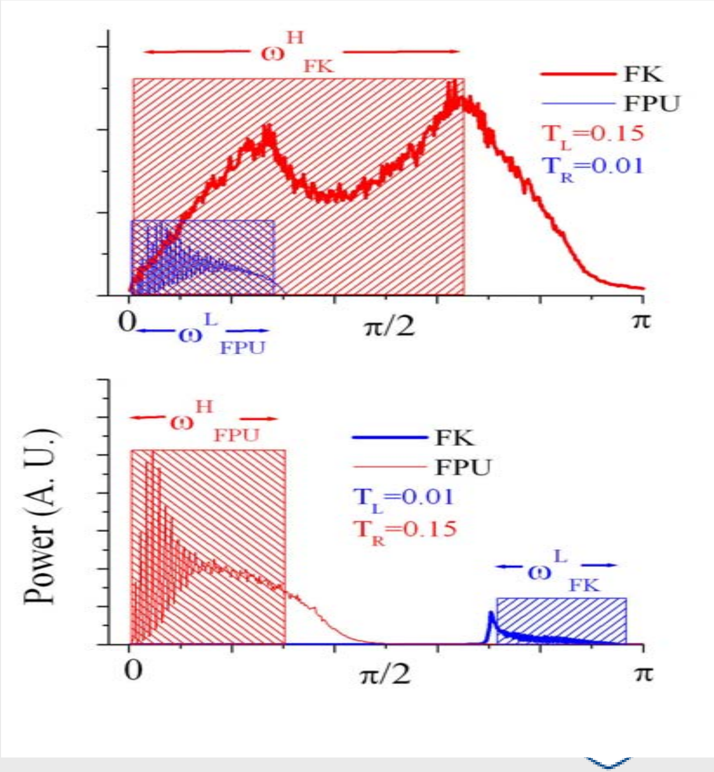
Thermal diode: Model II: FK + (an)harmonic lattice.

BL, J Lan,and L Wang, Phys. Rev. Lett. 95, 104302 (2005)



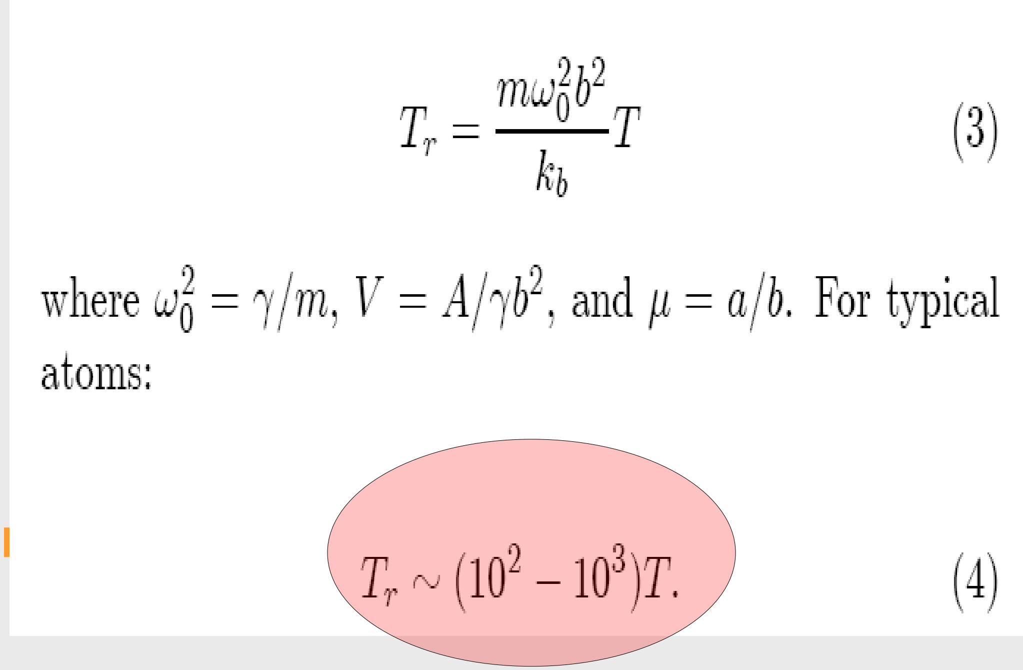






Possible nanoscale experiment

- **Temperature (simulation):**
- **$T \sim (0.1 \sim 1)$**
- **Real temperature**
- **$T_r \sim (10 \sim 100K)$**
- **System size:**
- Simulation: **N ~ (100-1000)**
- Real size: **(10-100nm)**
- Possible nanomaterials**: Nanotubes, Nanowires, Thin film ….**

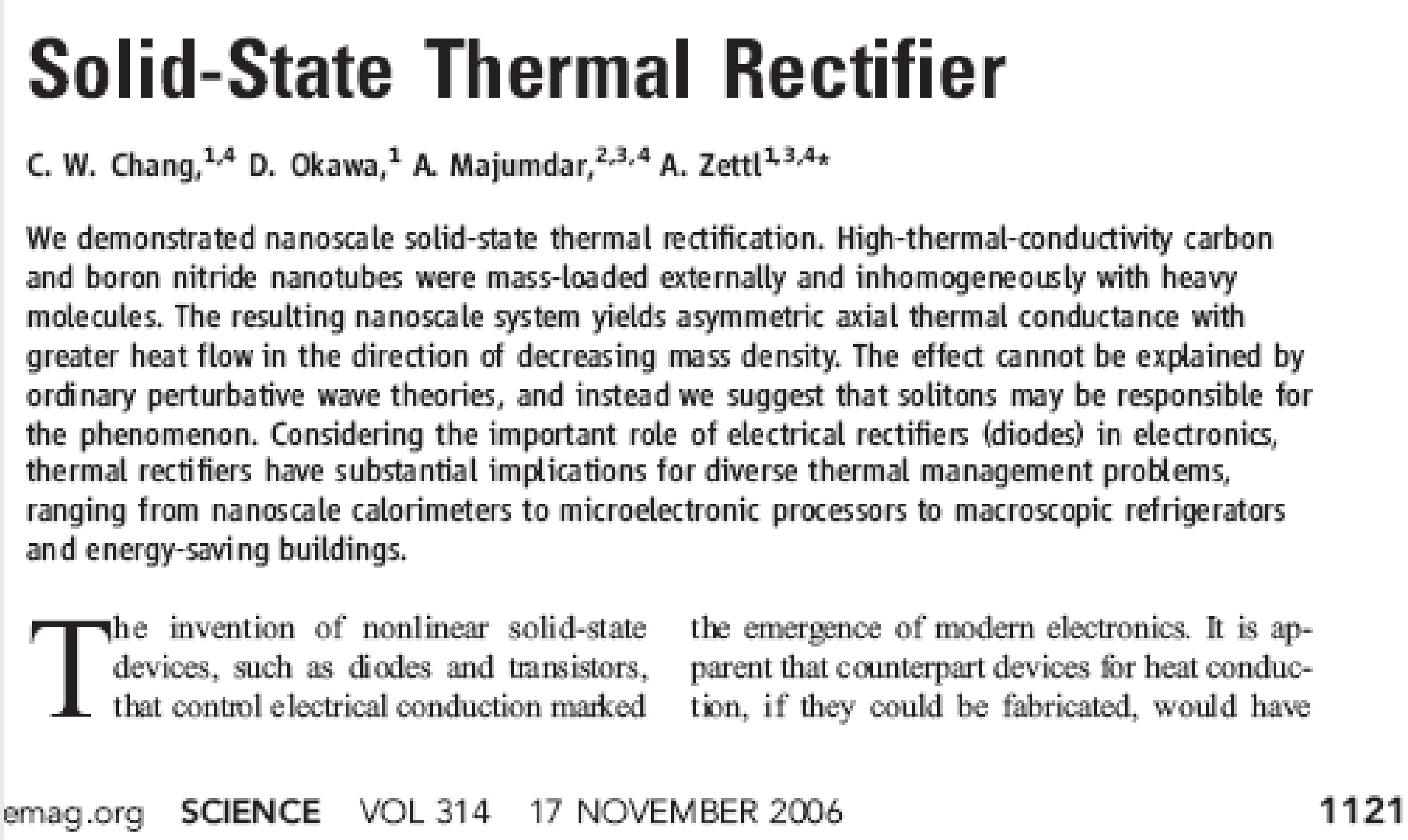


$$T_r = \frac{m\omega_0^2 b^2}{k_b} T \qquad (3)$$

where $\omega_0^2 = \gamma/m$, $V = A/\gamma b^2$, and $\mu = a/b$. For typical atoms:

$$T_r \sim (10^2 - 10^3)T. \qquad (4)$$

Nanoscale experiment of solid state thermal rectifier



Solid-State Thermal Rectifier

C. W. Chang,[1,4] D. Okawa,[1] A. Majumdar,[2,3,4] A. Zettl[1,3,4*]

We demonstrated nanoscale solid-state thermal rectification. High-thermal-conductivity carbon and boron nitride nanotubes were mass-loaded externally and inhomogeneously with heavy molecules. The resulting nanoscale system yields asymmetric axial thermal conductance with greater heat flow in the direction of decreasing mass density. The effect cannot be explained by ordinary perturbative wave theories, and instead we suggest that solitons may be responsible for the phenomenon. Considering the important role of electrical rectifiers (diodes) in electronics, thermal rectifiers have substantial implications for diverse thermal management problems, ranging from nanoscale calorimeters to microelectronic processors to macroscopic refrigerators and energy-saving buildings.

The invention of nonlinear solid-state devices, such as diodes and transistors, that control electrical conduction marked the emergence of modern electronics. It is apparent that counterpart devices for heat conduction, if they could be fabricated, would have

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Experiment’s Setup

Multi-walled BNNTs:

outer diameter: ~30 to 40 nm
length : ~10 µm.

Multi-walled CNTs:

outer diameter: ~10 to 33 nm
length : ~10 µm.

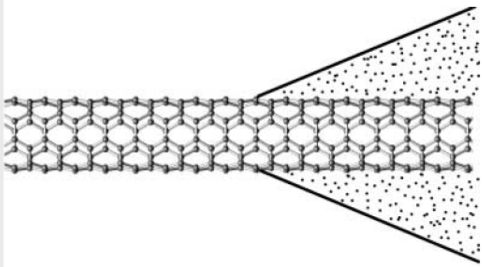
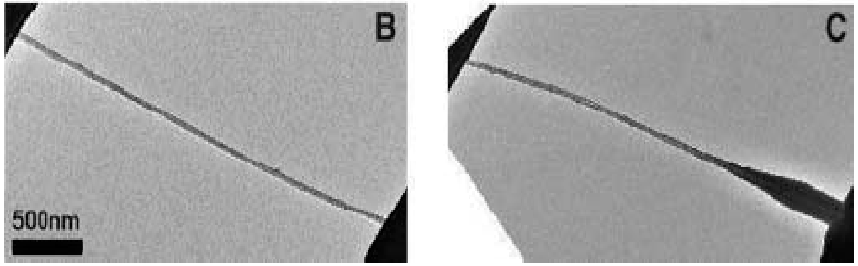


Fig. 1. A schematic description of depositing amorphous $C_9H_{16}Pt$ (black dots) on a nanotube (lattice structure).



TEM image

Before and After Deposition

The fixture incorporates independently SiNx pads, with symmetrically fabricated Pt film resistors serving as either heaters or sensors.

One end of the nanotube was bonded to the heater, the other end to the sensor, and the body of the nanotube was suspended in the vacuum.

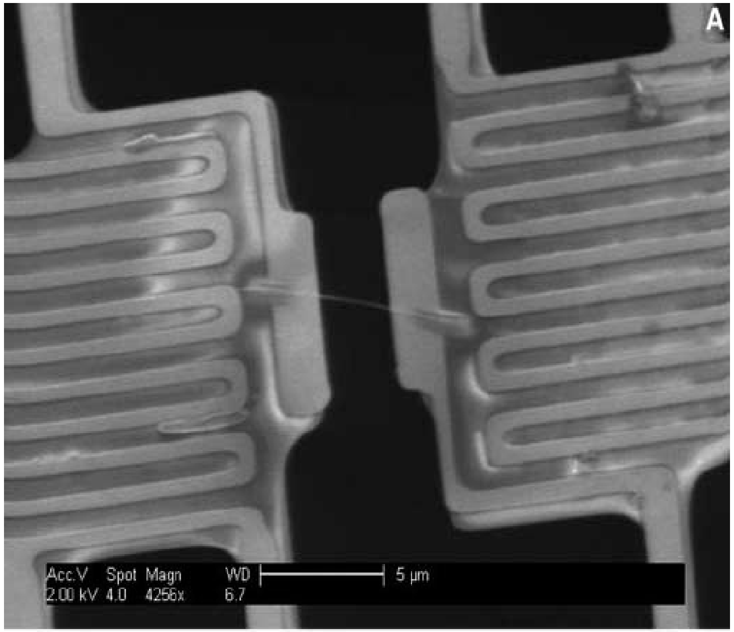


Fig. 2. (**A**) The SEM image of a CNT (light gray line in center) connected to the electrodes. Scale bar, 5 μm. (**B** and **C**) The corresponding low-magnification TEM images of the same CNT in (A), before (B) and after (C) $C_9H_{16}Pt$ was deposited.

Measurement of K

$$K = \frac{P}{\Delta T_h - \Delta T_s}\left(\frac{\Delta T_s}{\Delta T_h + \Delta T_s}\right) \qquad (1)$$

$$K = \frac{J}{\Delta T} = \frac{P2}{\Delta Th - \Delta Ts} \qquad (2)$$

$$P = P1 + P2, \qquad (3)$$

$$P2 = P3 \qquad (4)$$

$$P1 = C1 \cdot \Delta Th, \qquad (5)$$

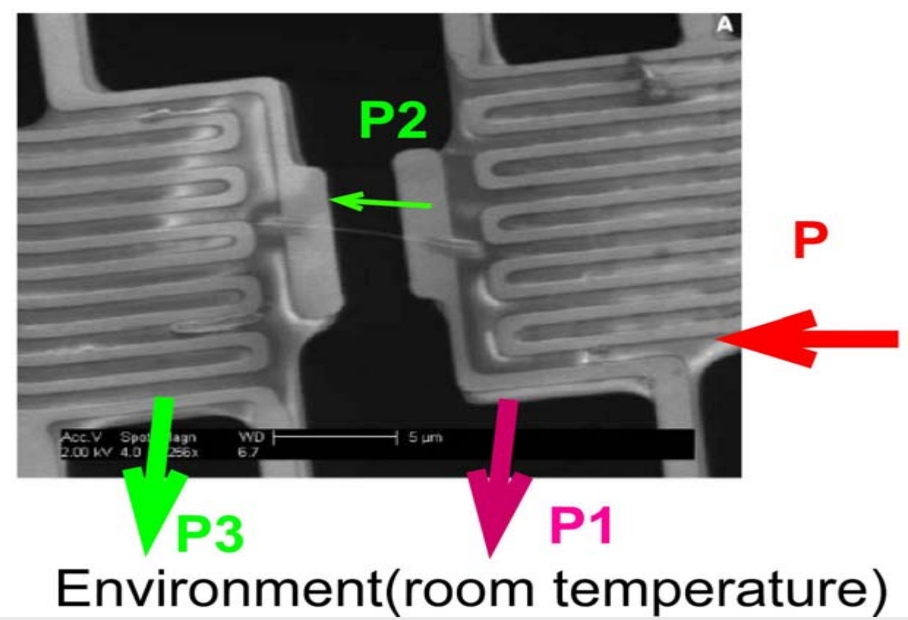
$$P3 = C2 \cdot \Delta Ts \qquad (6)$$

$$\text{Specific heat capacity}: C1 = C2 = C$$

$$(3)(4)(5)(6) \Rightarrow P = C(\Delta Th + \Delta Ts) \qquad (7)$$

$$(6)(7) \quad \Rightarrow P2 = P\Delta Ts/(\Delta Th + \Delta Ts) \qquad (8)$$

$$(8)(2) \quad \Rightarrow \quad (1)$$



Rectification

$$Rectification = \frac{K_{H\to L} - K_{L\to H}}{K_{L\to H}} \times 100\% \qquad (2)$$

- **A** higher **thermal** conductance **was observed when heat flowed from the** high-mass **region (where more C9H16Pt deposited) to the** low-mass **region.**

- **Rectification:**
  - CNT : **2%.**
  - Three different deposition BNNTs *Fig. 3 A to C* : **7%, 4%, and 3%.**

- **Comparison of conductances *Fig. 3 D***

$$Slope: s \equiv \Delta T_h / \Delta T_s << 1,$$

$$K = sP/\Delta T_h \left(1 - s^2\right) \approx sP/\Delta T_h$$

  - before deposition: no rectification
  - after deposition: rectification

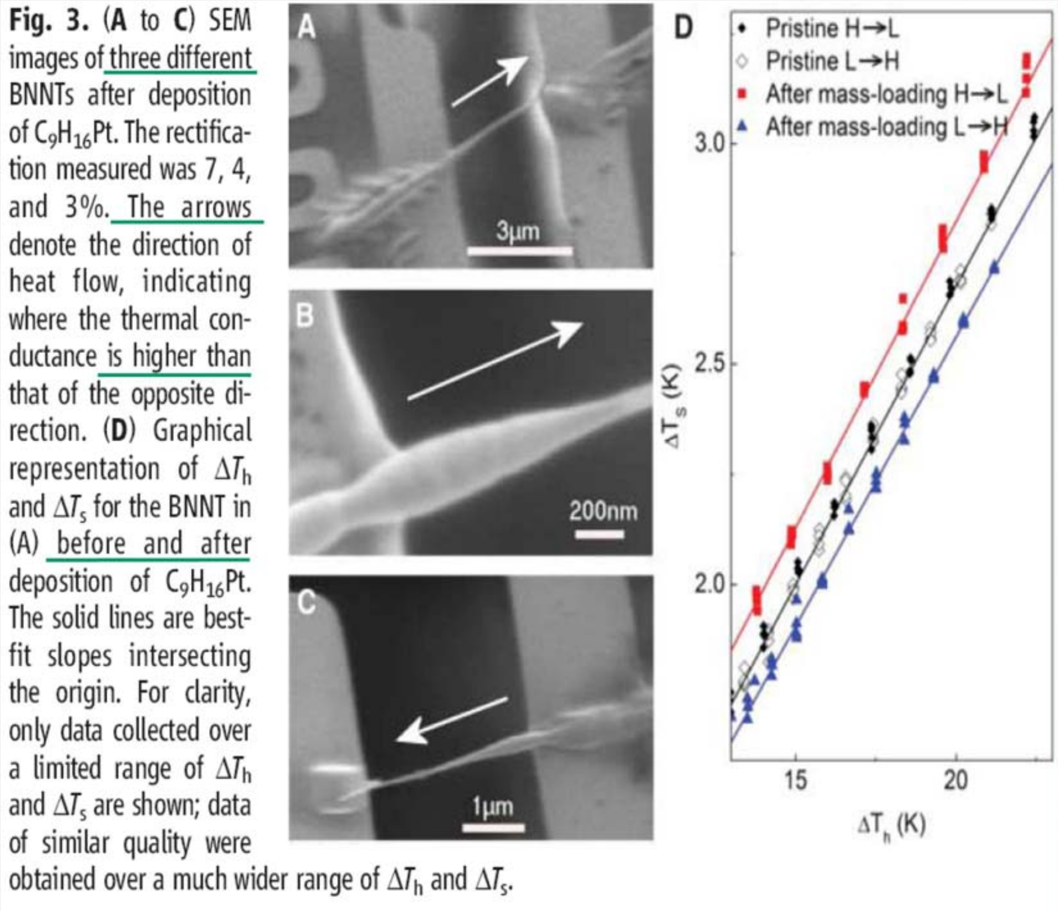


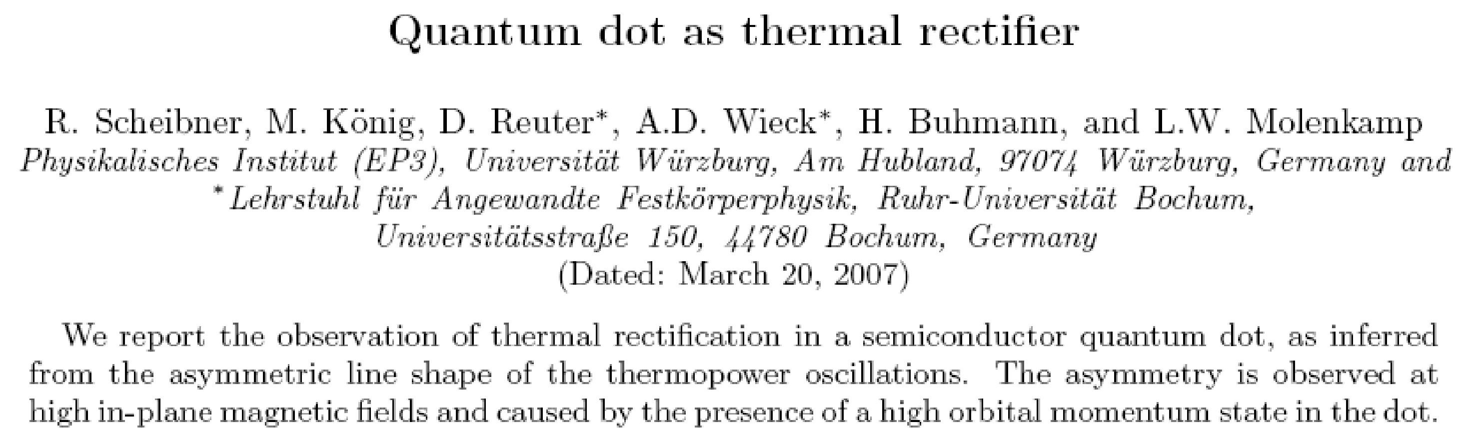
Fig. 3. (**A** to **C**) SEM images of three different BNNTs after deposition of $C_9H_{16}Pt$. The rectification measured was 7, 4, and 3%. The arrows denote the direction of heat flow, indicating where the thermal conductance is higher than that of the opposite direction. (**D**) Graphical representation of ΔT_h and ΔT_s for the BNNT in (A) before and after deposition of $C_9H_{16}Pt$. The solid lines are best-fit slopes intersecting the origin. For clarity, only data collected over a limited range of ΔT_h and ΔT_s are shown; data of similar quality were obtained over a much wider range of ΔT_h and ΔT_s.

Summary II

The 1D thermal rectifier has been demonstrated experimentally.

More works are expected to appear soon.

Quantum dot thermal rectifier (cond-mat/0701534)



Quantum dot as thermal rectifier

R. Scheibner, M. König, D. Reuter*, A.D. Wieck*, H. Buhmann, and L.W. Molenkamp
Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany and
**Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum,*
Universitätsstraße 150, 44780 Bochum, Germany
(Dated: March 20, 2007)

We report the observation of thermal rectification in a semiconductor quantum dot, as inferred from the asymmetric line shape of the thermopower oscillations. The asymmetry is observed at high in-plane magnetic fields and caused by the presence of a high orbital momentum state in the dot.

Part I: Heat conduction in single walled nanotubes:

Simulation and Experiment

Part II: Computation with Phonons

2.1	Thermal diode/rectifier: rectification of heat flux Simulation and Experiment
2.2	Thermal Transistor: heat switch and modulator
2.3	Thermal logic gate

Transistor: switching and Amplification
Bipolar Transistor (Barden and Brattain)

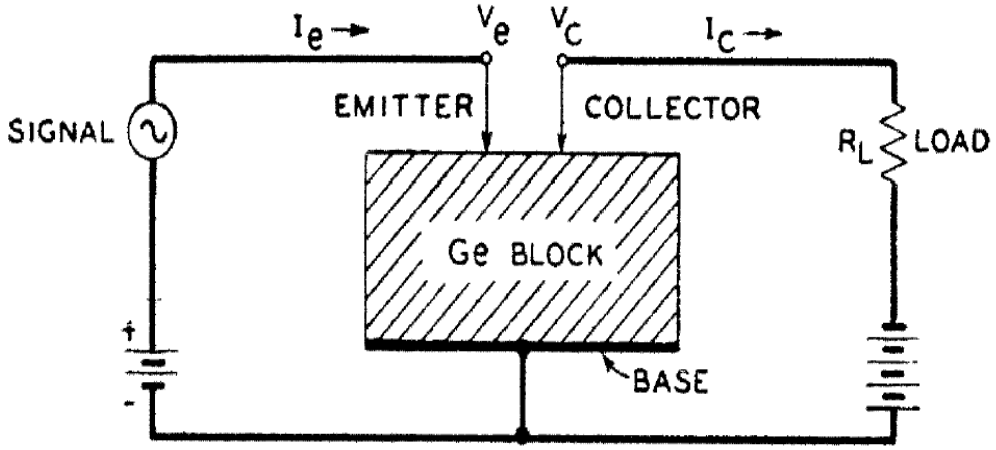
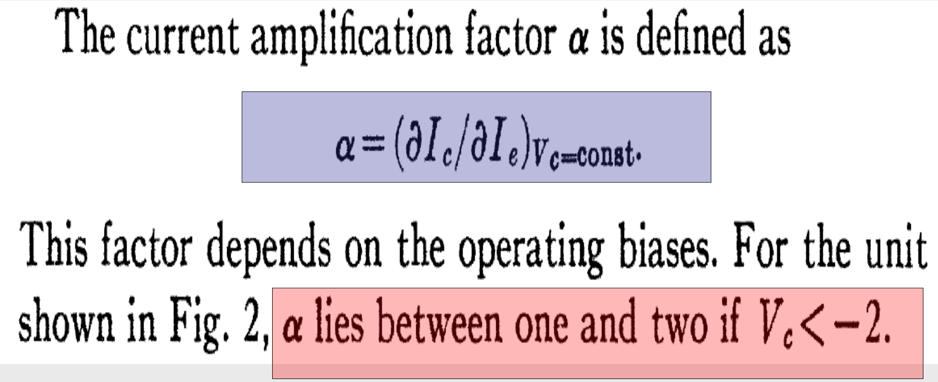


FIG. 1. Schematic of semi-conductor triode.

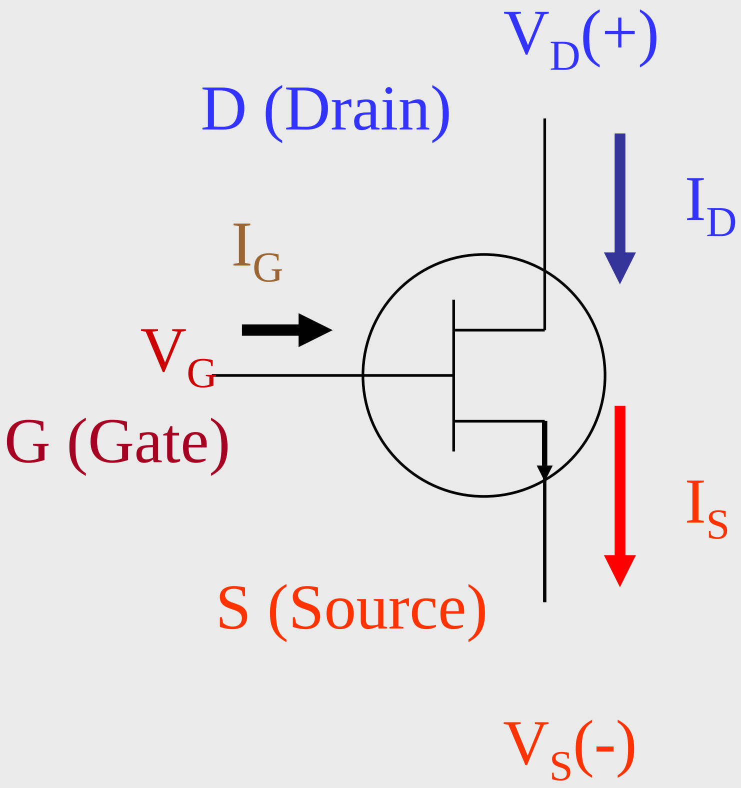


The current amplification factor α is defined as

$$\alpha = (\partial I_c/\partial I_e)_{V_c=\text{const}}.$$

This factor depends on the operating biases. For the unit shown in Fig. 2, α lies between one and two if $V_c < -2$.

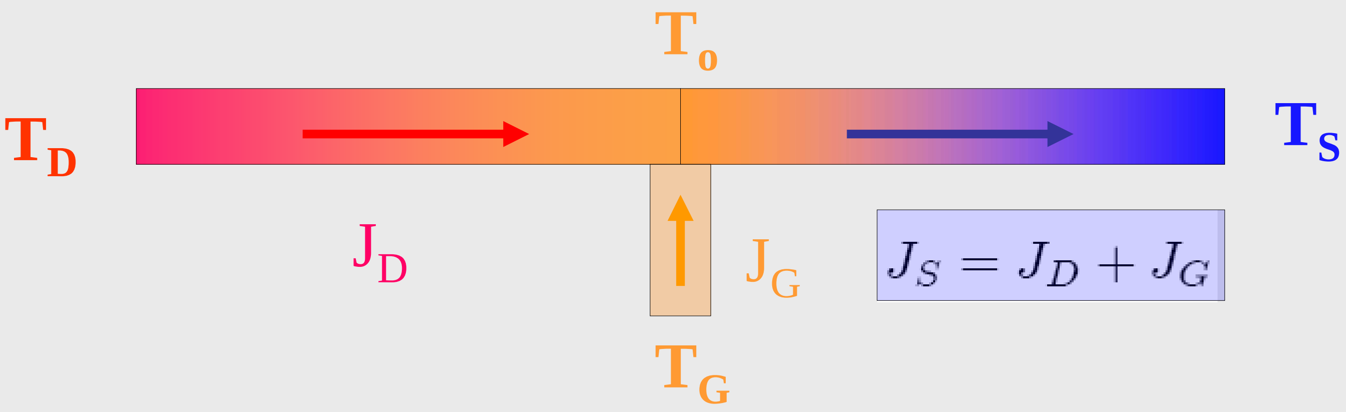
MOSFET



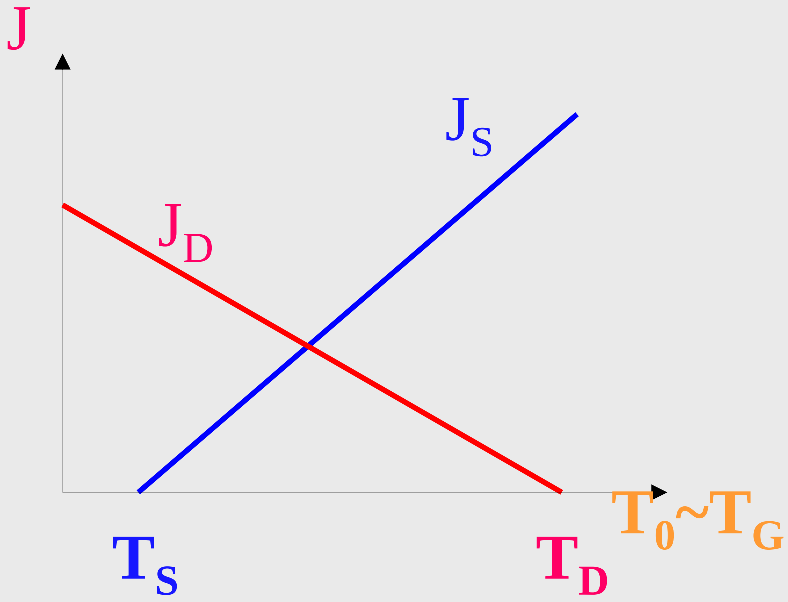
$I_G \approx 0,$

$I_D \approx I_S$

How to build a thermal transistor ?



$$J_S = J_D + J_G$$



Differential thermal resistance:

$$R_S = \left(\frac{\partial J_S}{\partial T_o}\right)^{-1}_{T_S=\text{const}}$$

$$R_D = -\left(\frac{\partial J_D}{\partial T_o}\right)^{-1}_{T_D=\text{const}}$$

Current amplification:

$$\alpha = \left| \frac{\partial J_D}{\partial J_G} \right| = \left| \frac{R_S}{R_S + R_D} \right| < 1$$

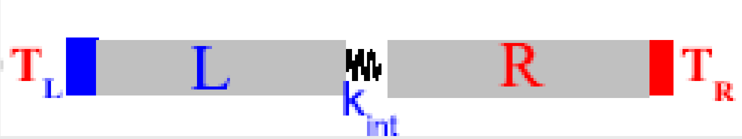
The thermal transistor never works !!!

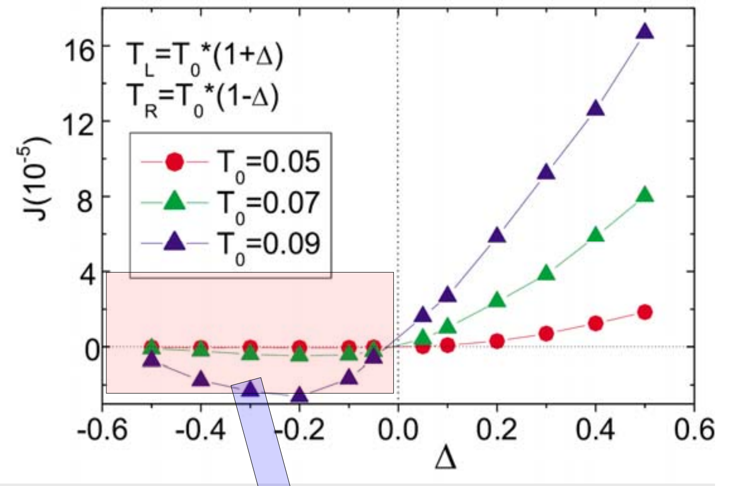
Think something differently!!!

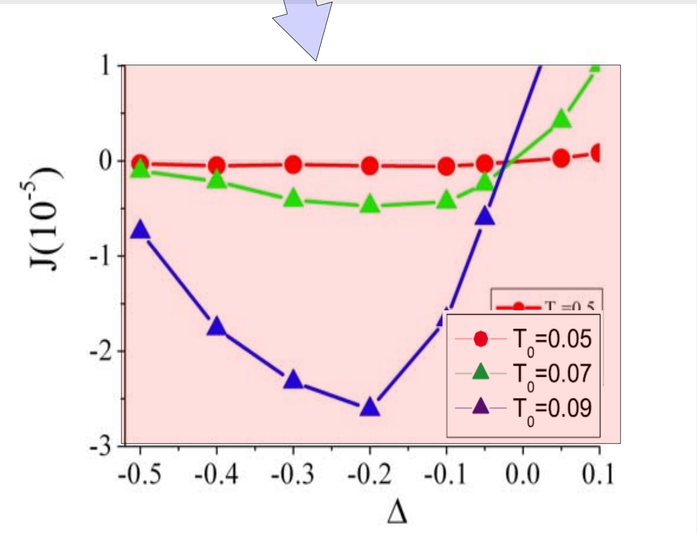
$$\alpha = \left|\frac{\partial J_D}{\partial J_G}\right| = \left|\frac{R_S}{R_S + R_D}\right|$$

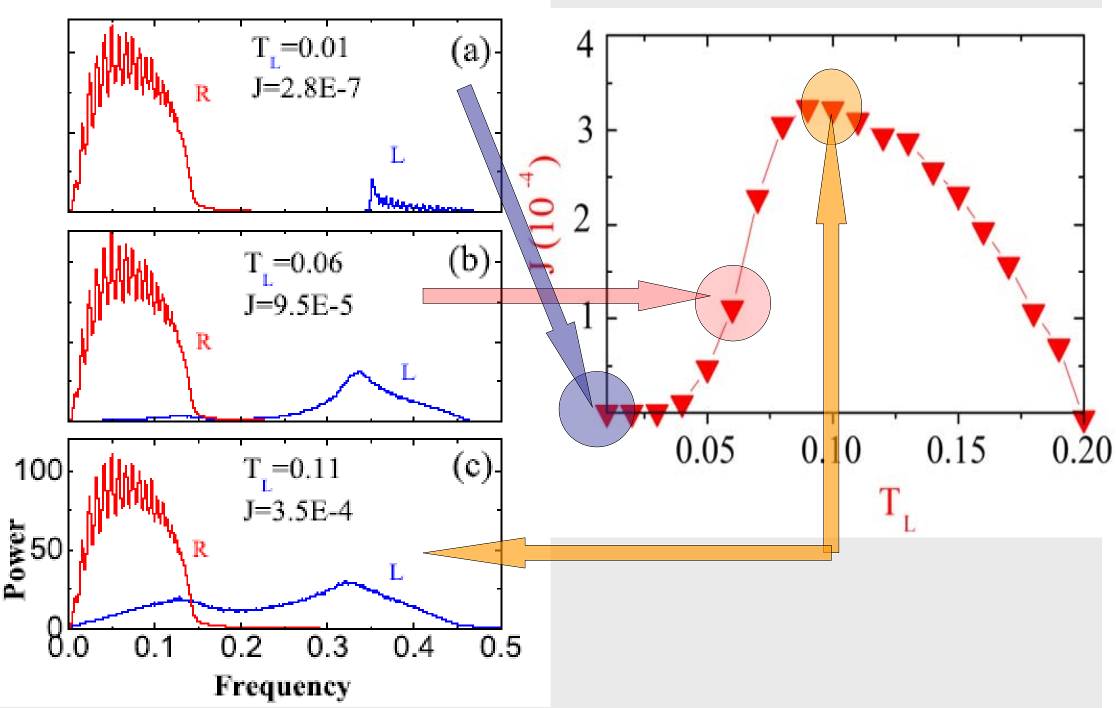
How about if one of
the differential thermal resistance is negative?

Negative differential thermal resistance /conductance



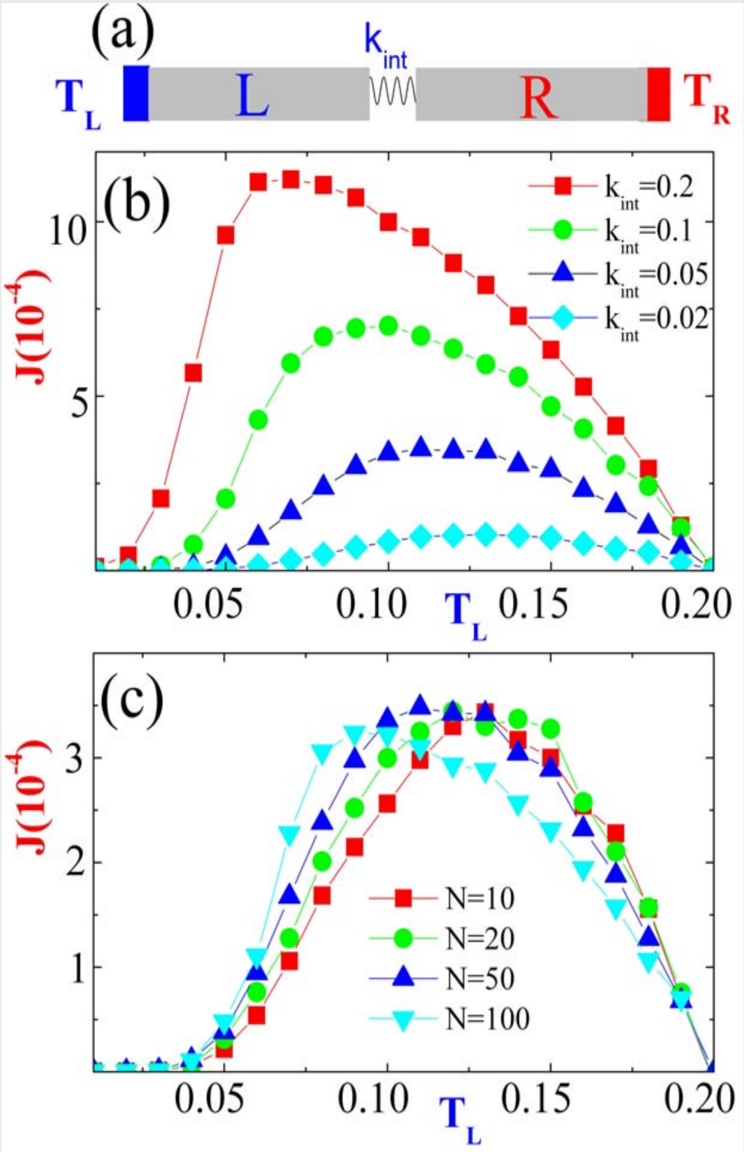






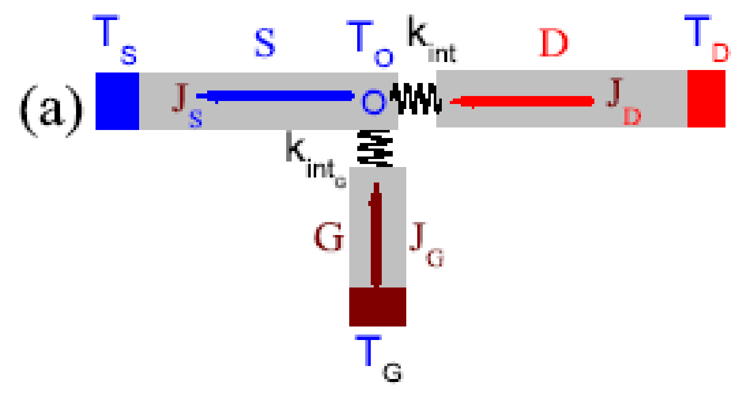
Negative Differential Thermal Resistance/Conductance

BL, L Wang, and G Casati, *Appl. Phy. Lett* 88, 143501 (2006).

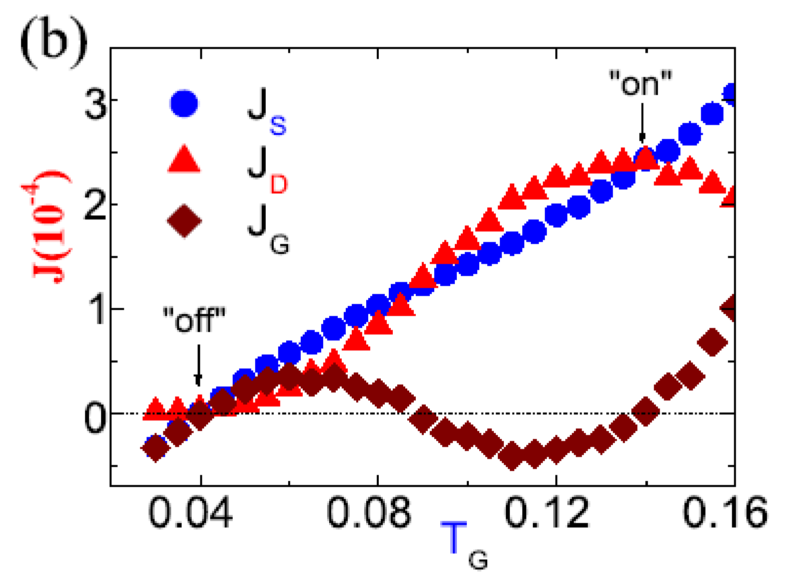


Thermal transistor

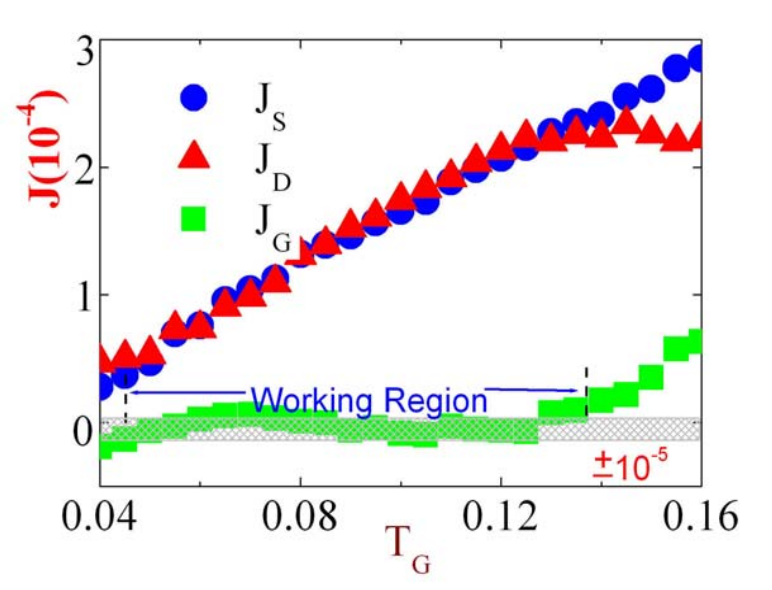
BL, L Wang, and G Casati, *Appl. Phy. Lett* 88, 143501 (2006).



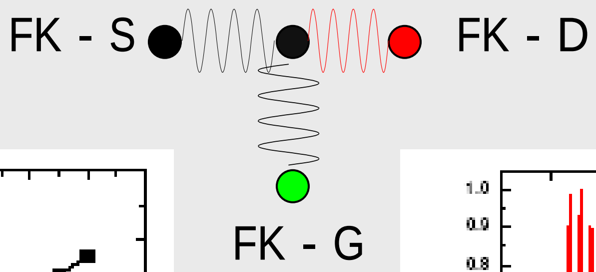
Function 1: Switch

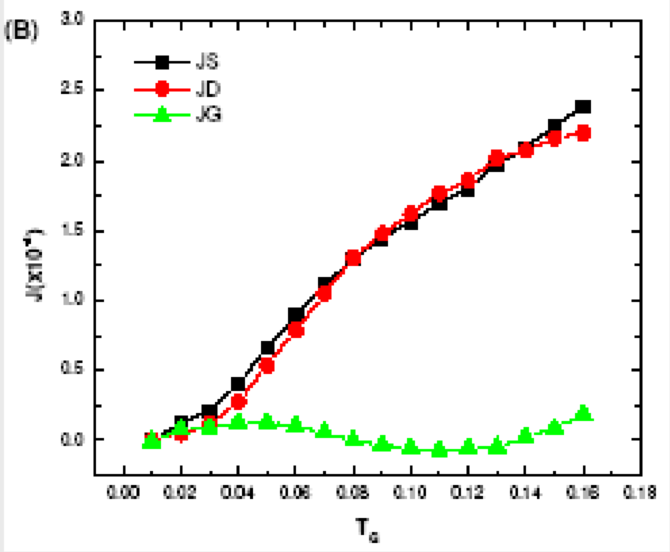


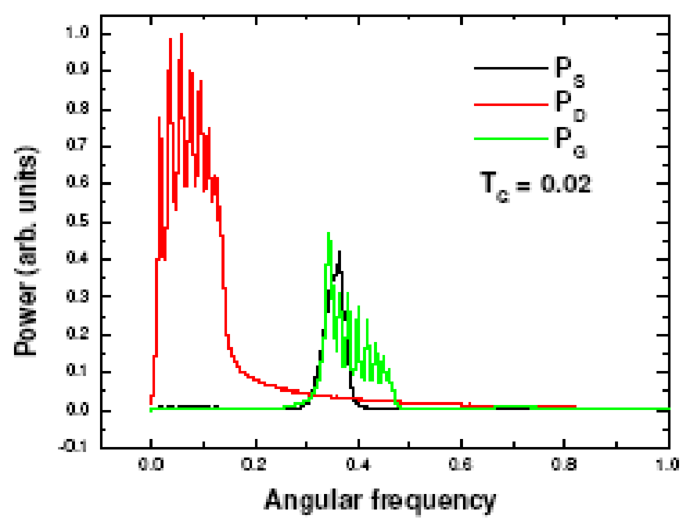
Function 2: modulator/amplifier

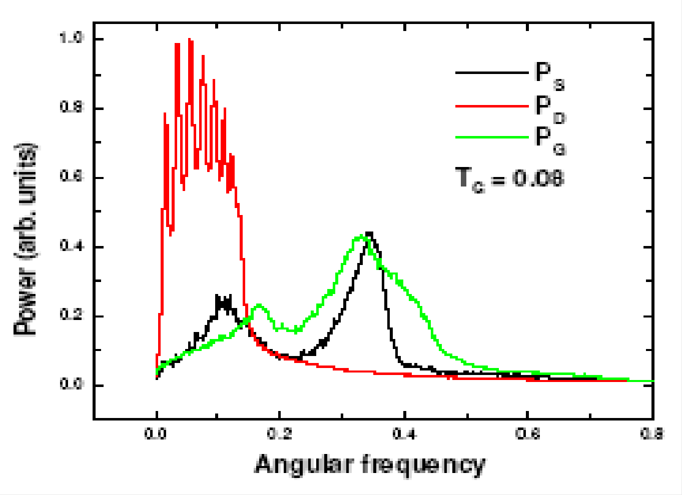


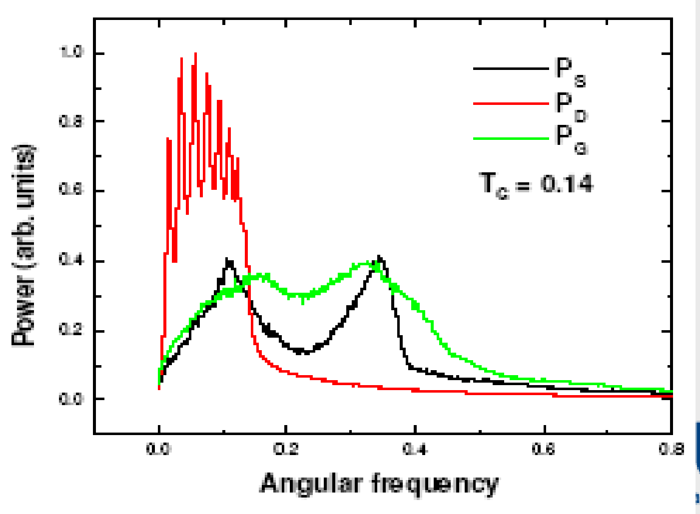
T_G=.04, .09, .14, J_G=0, J_D=2.4e-6, 1.1e-4, 2.3e-4


FK - S
FK - D
FK - G


(B)
JS
JD
JG
J(x10^-4)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
T_G


P_S
P_D
P_G
T_G = 0.02
Power (arb. units)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
0.0
0.2
0.4
0.6
0.8
1.0
Angular frequency


P_S
P_D
P_G
T_G = 0.08
Power (arb. units)
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
Angular frequency


P_S
P_D
P_G
T_G = 0.14
Power (arb. units)
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
Angular frequency

Part I: Heat conduction in single walled nanotubes:

Simulation and Experiment

Part II: Computation with Phonons

2.1 Thermal diode/rectifier: rectification of heat flux
Simulation and Experiment
2.2 Thermal Transistor: heat switch and modulator
2.3 Thermal logic gates

NUS
National University of Singapore

Thermal logic gates: computation with phonons

L Wang and BL, Phys. Rev. Lett. 99, 177303 (2007) (24 October 2007)

- **Repeater**
- **NOT gate**
- **AND /OR Gate**

Media reports

Physics New Updates (AIP)

Physical Review Focus (APS)

Phys Org

Dark Net

Solidot (Chinese)

Only Perception (Taiwan)

Lenta (Russia)

Daily Science News

Physics World (feature article)

....

....

Transistor

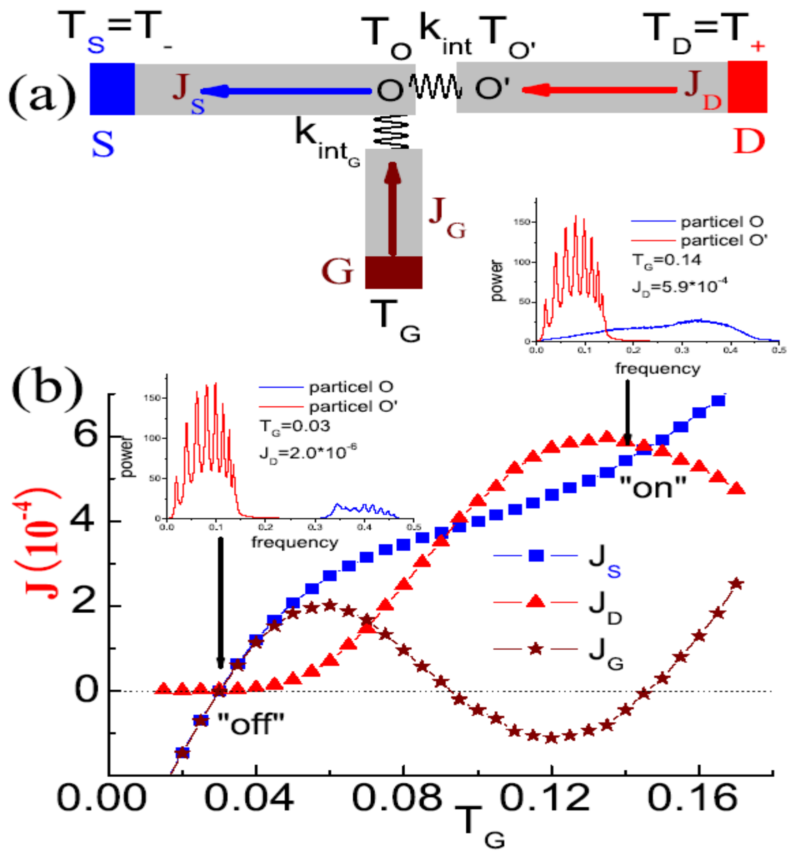
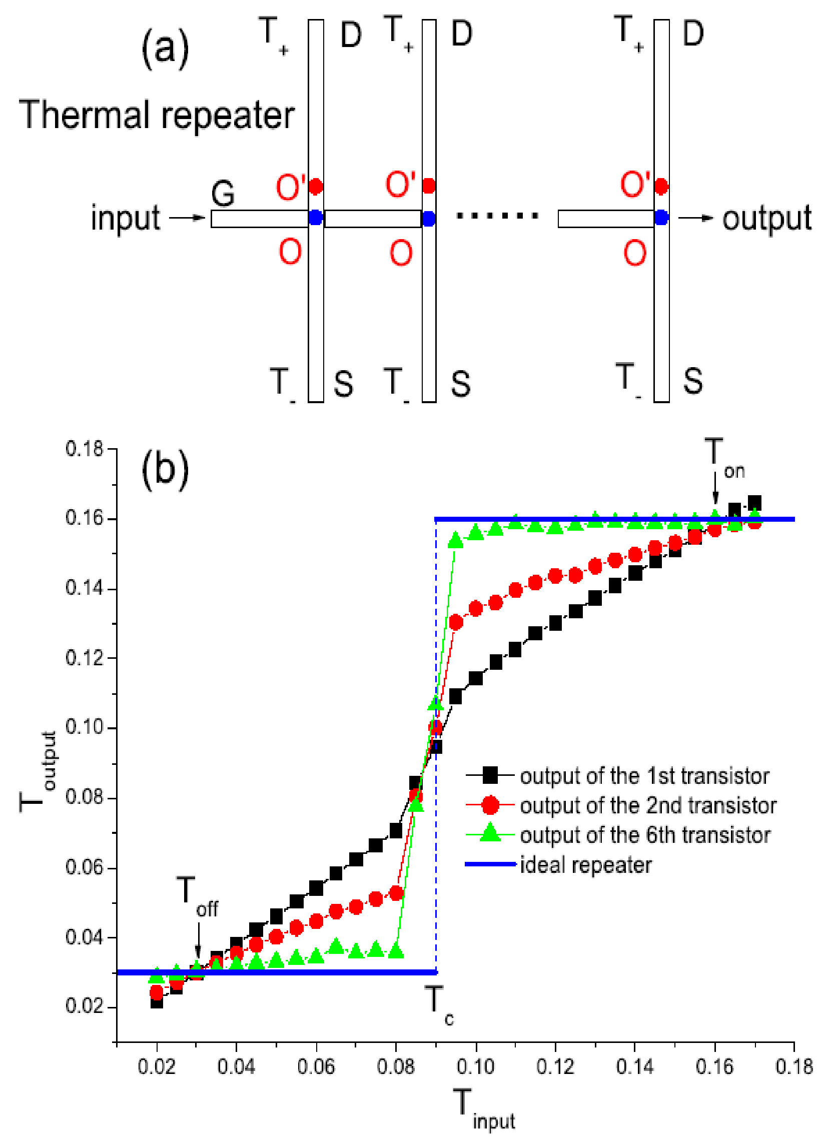


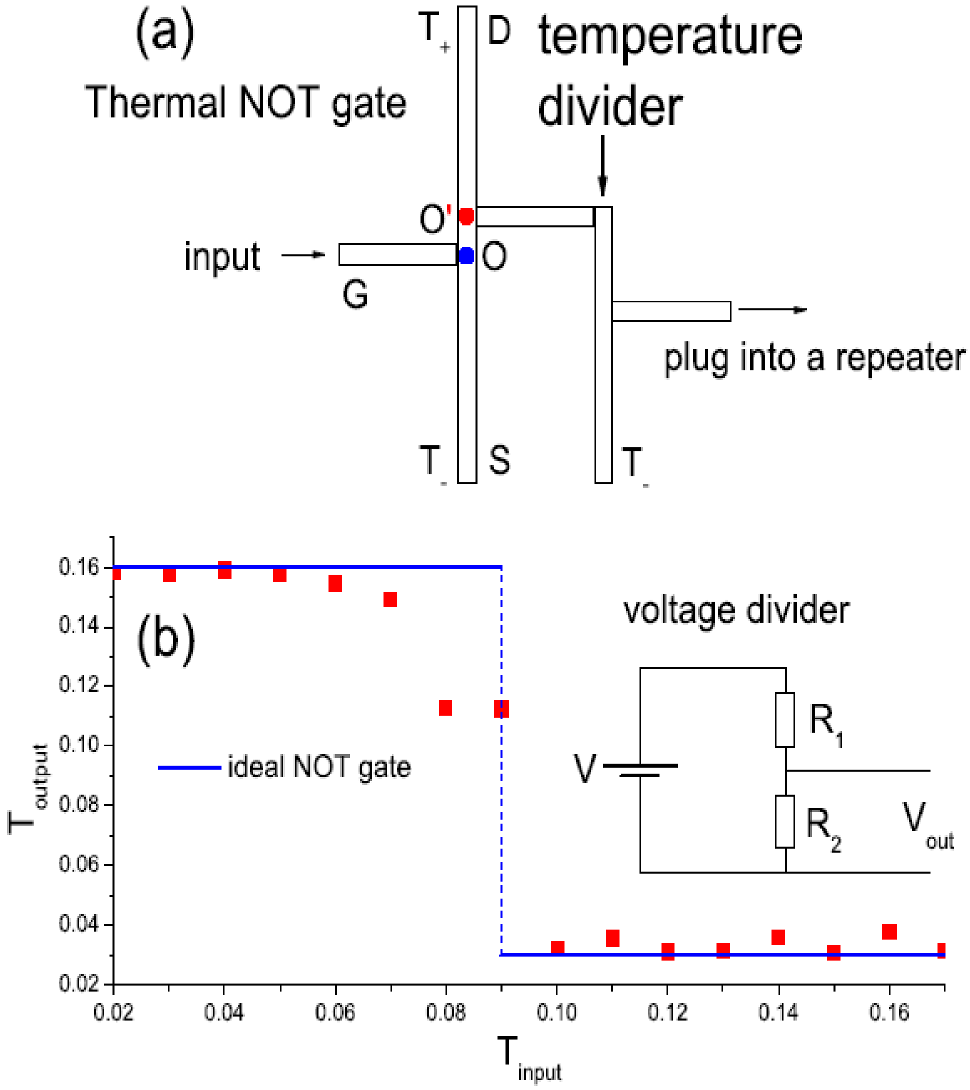
FIG. 1: (a) Configuration of the thermal transistor. (b) Heat currents through three terminals D, S and G versus temperature T_G. Notice the NDTR effect that in a wide region both J_S and J_D increase when temperature T_G is increased. At T_G=T_{on} and T_{off}, thus J_G is exactly zero. Insets: power spectra of particles O and O' near 'off' and 'on' states. Power spectrum of O depends on temperature sensitively. It matches that of O' much better at 'on' state than at 'off' state, which makes J_D is much higher at 'on' state although temperature difference between terminal D and particle O is much larger at 'off' state.

Signal Repeater

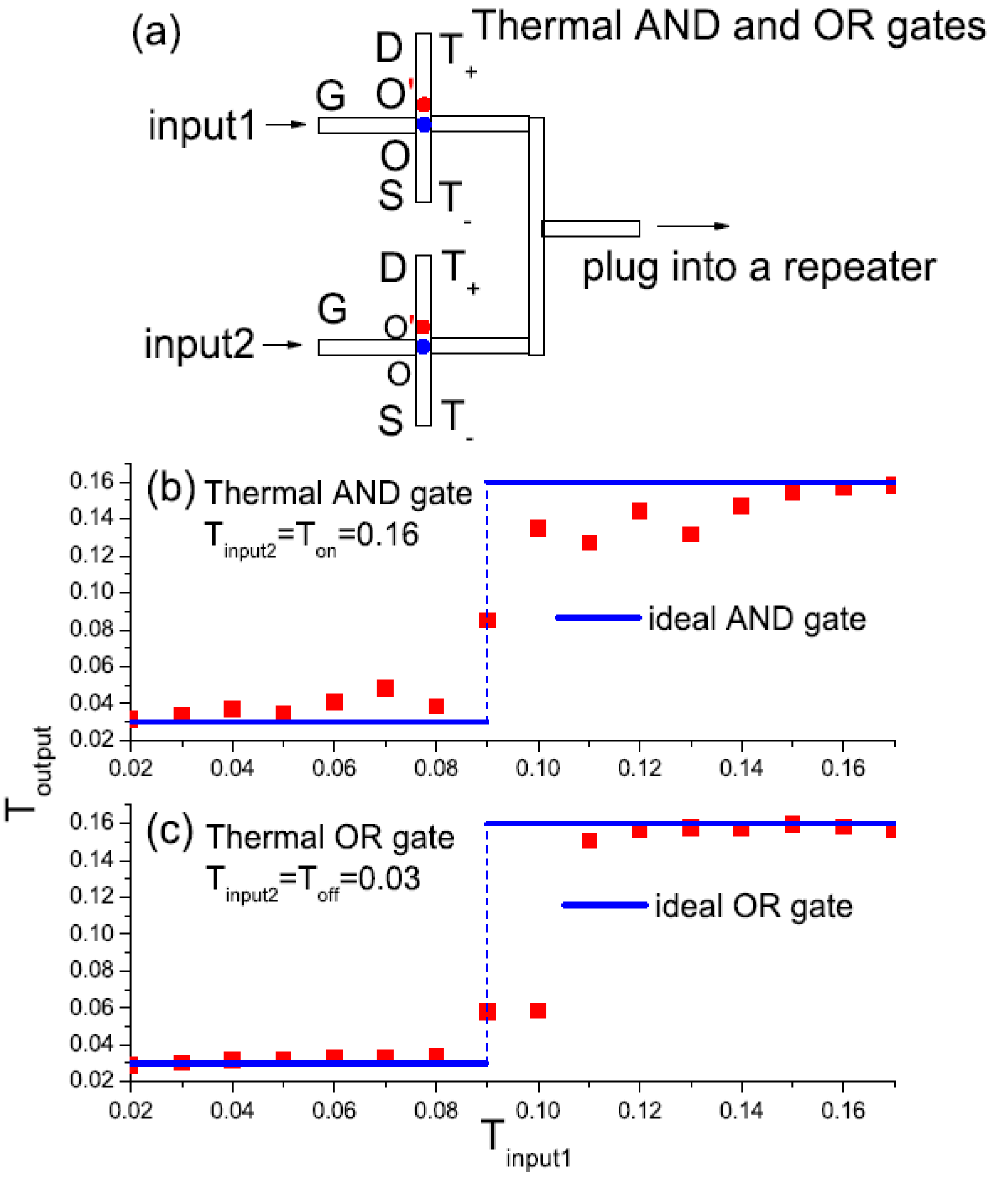
$$\begin{cases} T_{output} = T_{off}, & \text{if} \quad T_{input} < T_c, \\ T_{output} = T_{on}, & \text{if} \quad T_{input} > T_c. \end{cases}$$



NOT Gate


(a)
Thermal NOT gate
T+
D
temperature divider
O'
input
G
O
plug into a repeater
T-
S
T-
(b)
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
ideal NOT gate
voltage divider
V
R1
R2
Vout
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
Toutput
Tinput

AND/OR Gate


(a)
Thermal AND and OR gates
input1
input2
G
D
S
O
O'
T+
T-
plug into a repeater
(b) Thermal AND gate
$T_{input2}=T_{on}=0.16$
ideal AND gate
(c) Thermal OR gate
$T_{input2}=T_{off}=0.03$
ideal OR gate
T_{output}
T_{input1}
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16

Take Home Message

1. **Rectifying effect is very generic in nonlinear lattices.**
2. **Solid state thermal rectifier is feasible in (meso) nano scale systems.**
3. **A thermal transistor can be built with the *negative differential thermal resistance*.**
4. **Heat (phonon) computation is in principle possible.**

Acknowledgement

Collaborators

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Dr. WANG Lei (NUS)
Dr. WANG Jiao (Temasek Lab,NUS)
Dr. LAN Jing-hua (NUS, IHPC/A*STAR)
Mr. LO Weichung (NUS, IHPC/A*STAR)
Prof. Giulio CASATI (NUS/Como, Italy)

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Ministry of Education, Singapore
Faculty Research Grant, NUS

BL's Group:

30+ members from 11 countries.

Singapore, Malaysia, China, India, Germany, Italy, Spain, Denmark, Turkey, Cuba, USA.

Relevant publications

Thermal Logic gate

L Wang and B Li, *Phys. Rev. Lett,* 99, 177208 (2007),

(AIP/APS Physics News Update #840-2. Physical Review Focus)

Thermal transistor

B Li, L Wang and G Casati, *Appl. Phys. Lett*. 88, 143501 (2006).

Thermal diode/rectifier

B Li, L Wang, and G Casati, *Phys. Rev. Lett*. 93, 184301 (2004)

B Li, J-H Lan, and L Wang, *Phys. Rev. Lett,* 95, 104302 (2005) .

G. Wu and B. Li, *Phys. Rev. B* 76， 085424 (2007).

J.-H Lan and B Li, *Phys. Rev. B* 74, 214305 (2006); 75, 214302 (2007)

N. Yang, N.- B Li, L Wang, and B Li, *Phys. Rev. B* 76, 020301 (R) (200

Relevant publications (cont.)

Heat conduction in nanotubes

G Zhang and B Li, *J. Chem. Phys*. 123, 114714 (2005)

G Zhang and B Li, *J. Chem Phys*. 123, 014705 (2005).

Z.-H Yao, J.-S Wang and B Li, *Phys. Rev. B* 71, 085417 (2005)

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Anomalous diffusion

B Li, J Wang, L Wang and G Zhang, *CHAOS*, 15, 015121(2005)

B Li and J Wang, *Phys. Rev. Lett* 91, 044301 (2003); 92, 089402 (2004)

Relevant publications (cont.)

Heat conduction in one dimensional systems

Effective Phonon Theory

N.-B Li and B. Li, *Phys Rev E* 76， 011108 (2007)
N.-B Li and B. Li, *EPL* 78, 3400 (2007) .
N.-B Li, P.-Q Tong, and B Li. *Europhs Let* 75, 49-55 (2006).

Mode Coupling Theory

J.-S Wang and B Li, *Phys. Rev. E* 70, 021204 (2004)

J.-S Wang and B. Li, *Phys. Rev. Lett.* 92, 074302 (2004)

Pure Numerical Works

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B Li, G Casati, J Wang, and T Prosen, *Phys. Rev. Lett*. 92, 254301 (2004)

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B Li, H Zhao, and B Hu *Phys. Rev. Lett* 87, 069402 (2001); 86, 63 (2001).
B. Hu, B Li, and H Zhao, *Phys. Rev. E* 61, 3828 (2000)
A Fillipov, B Hu, B Li and A. Zeltser, *J. Phys. A* 31, 7719 (1998).
B. Hu, B Li, and H Zhao, *Phys. Rev.* E 57, 2992 (1998)

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http://www.cse.nus.edu.sg/~tiencs2008