Thermo-electric modeling of Nano-Tube and Nano-Bridged Based Environmental Sensing

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Overview of Talk

- Motivation
- Simplified 1-D Models
- Nanotube Results
- Conclusions and Future Work

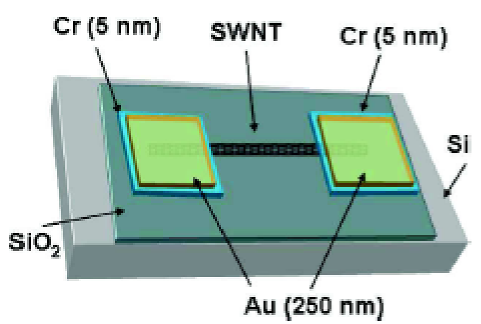
Motivation

•Quick over-view of summer work:

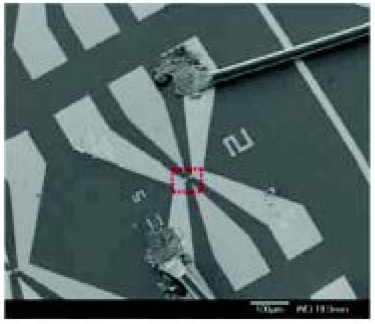
- Ongoing relationship (since Summer 2009) with Microdevices Laboratory (MDL), working on analysis and simulation of micro-device design for extreme (high heat flux, high temperature, high pressure) conditions.
- Previous topics include nanofluid heat transfer, design of radiation resistant nano-mechanical memory.
- Summer 2012 tasks included:
  - Analysis of thermo-electric coupling of suspended nanowire and bridge structures (topic today)
  - New configurations for electronics in harsh environments.
  - Support group in other tasks.

Motivation

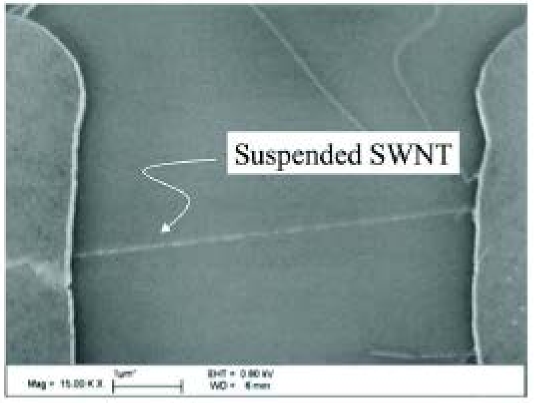
- Suspended nanowires are of interest for electronics applications, including field-emission devices and pressure sensors.
- Experimental measurements show that the electrical resistance of a suspended CNT is pressure-dependent
  - Effect must be *quantified* for most structures, but can be *exploited* to make pressure sensors.



Device Layout



Actual Device



Suspended nanotube

A. P. Kaul and H. M. Manohara, *IEEE Trans. on Nanotechnology* **8** 252, 2009.

Motivation

- Challenge: Can we combine all of the physics into a single simulation that predicts the physical behavior of these systems?
- Need to include:
  - Pressure-dependent convection coefficients
  - Temperature-dependent thermal conductivity and resistivity
  - Joule heating
  - Heat transfer into substrate
- Problem lends itself to numeric solution.

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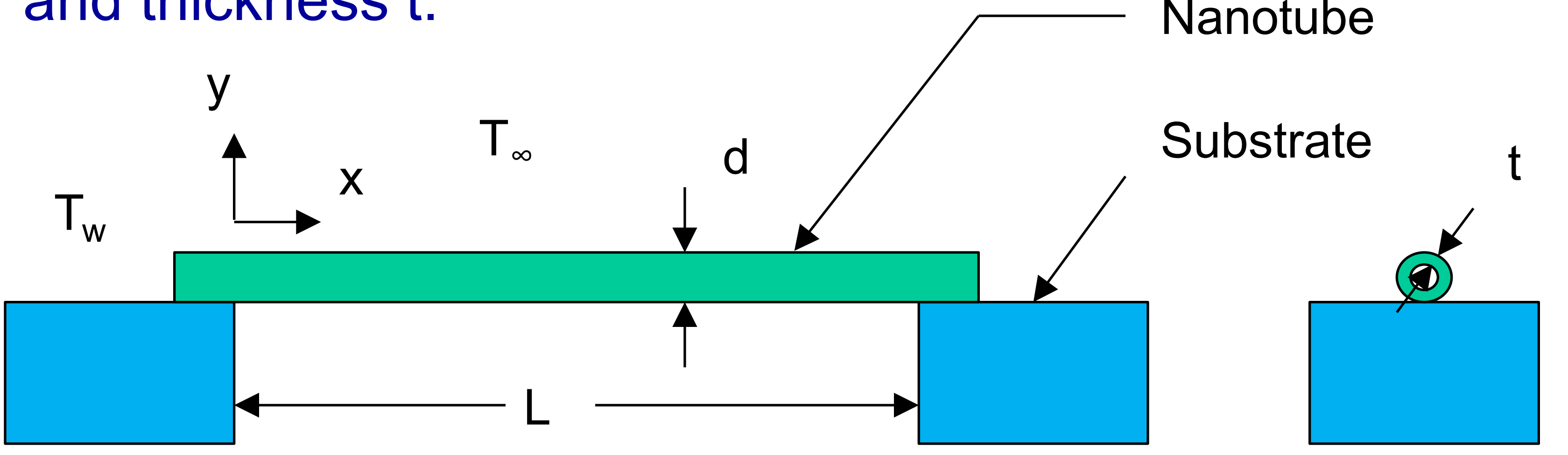
Numeric Formulation

- Model the nanotube as a structure of length L, diameter d, and thickness t.



- Heat is generated inside the nanotube, and lost to either the substrate or the ambient gas.

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- Since d is 1.3 nm, and L is 5 µm, the system will be one-dimensional, or $T = T(x)$.

Numeric Formulation

- The governing equation will be the conduction equation:

$$A_c \cdot k \cdot \frac{d^2T}{dx^2} - \mathrm{h} \cdot P \cdot [T(x) - T_\infty] + q_i = 0$$

A_c = Cross-sectional area
k = Thermal conductivity
h = Convective heat transfer coefficient
T_∞ = Ambient temperature
P = Perimeter
q_i = Joule heating per length

- q_i found from current, resistance:

$$q_i = \rho_r \cdot I^2 / A_c$$

ρ_r = Electrical resistivity
I = Electrical current

Numeric Formulation

- Electrical resistivity ρ_r and thermal conductivity k are functions of temperature:

$$\rho_r(T) = A_o + A_1 \cdot T + A_2 \cdot T^2$$

$$k(T) = B_o + B_1 \cdot T + B_2 \cdot T^2$$

  - Boundary condition at the end incorporates contact resistance $R_{t,c}''$

$$k \cdot \left.\frac{dT}{dx}\right|_{x=0} = \frac{T(x=0) - T_w}{R''_{t,c}}$$

- Either use same condition at x = L, or symmetry.

Numeric Formulation

- Flow physics determined by the Knudsen number:

$$Kn_d = \lambda / d$$

where λ is the mean free path of the gas molecules (~50 nm at atmospheric pressure, and inversely proportional to density).

•Kn > 10 indicates free-molecular flow.   Since a nanotube diameter d is around 1.3 nm, this is free molecular even at atmospheric pressure. h will then depend on the pressure P:

$$h = \sigma_t \cdot \left(\frac{\gamma + 1}{\gamma - 1}\right) \cdot P \cdot \sqrt{\frac{k_b}{8 \cdot \pi \cdot T_{gas} \cdot m_{gas}}}$$

σ_t = Thermal accommodation coeff. γ = Specific heat ratio

K_b = Boltzmann Constant m_{gas} = mass of molecule

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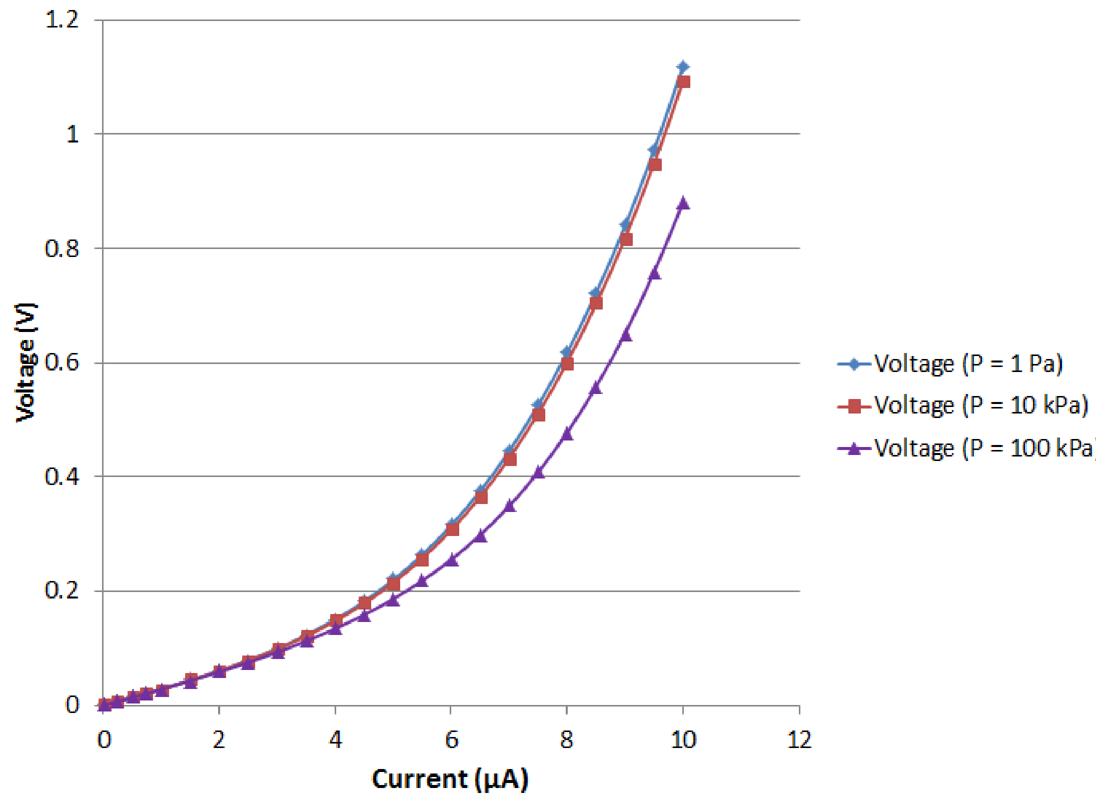
Results

- Simulated 5 µm long single-wall nanotube with no contact resistance to find heat dissipation, temperature as a function of current.

- Integrate resistance to get net voltage drop across system.

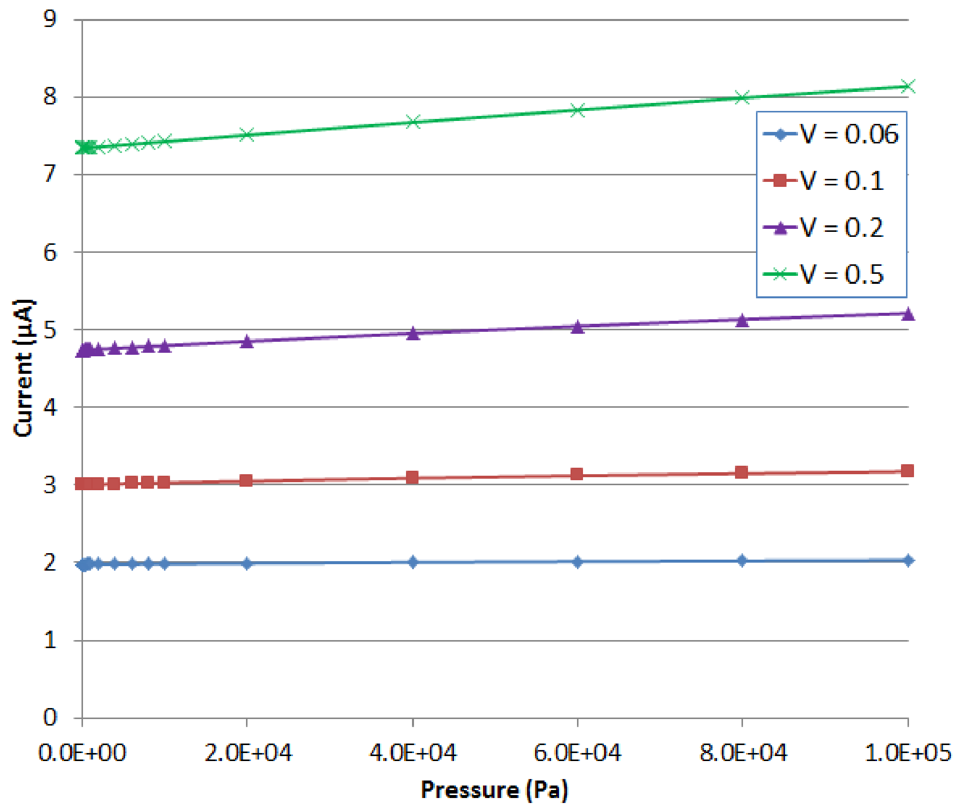


V vs. I for 5 µm long suspended nanotube

- 1) The temperature change due to heating changes the electrical resistance, making the curve non-linear.
  2) This effect is pressure-sensitive.

Results

- Current required to maintain a constant voltage at different pressures:
- Results confirm previous work that shows this can be a pressure-sensing mechanism.
- Alternative to Pirani gauges currently used.



I vs P for 5 μm long suspended nanotube

Results

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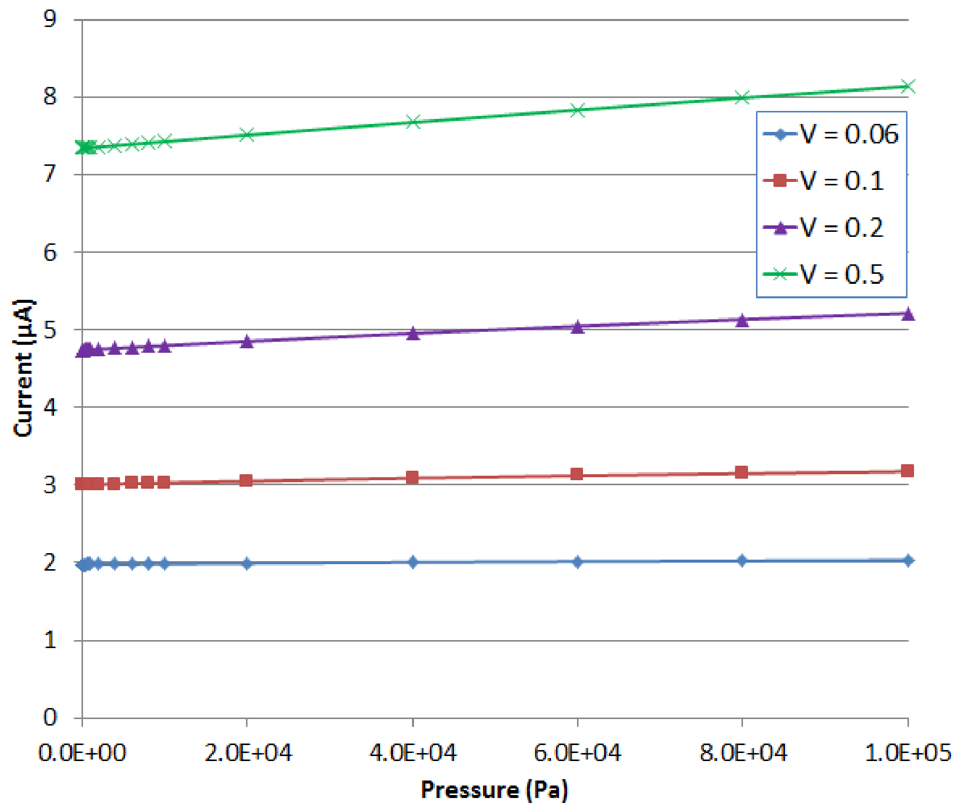
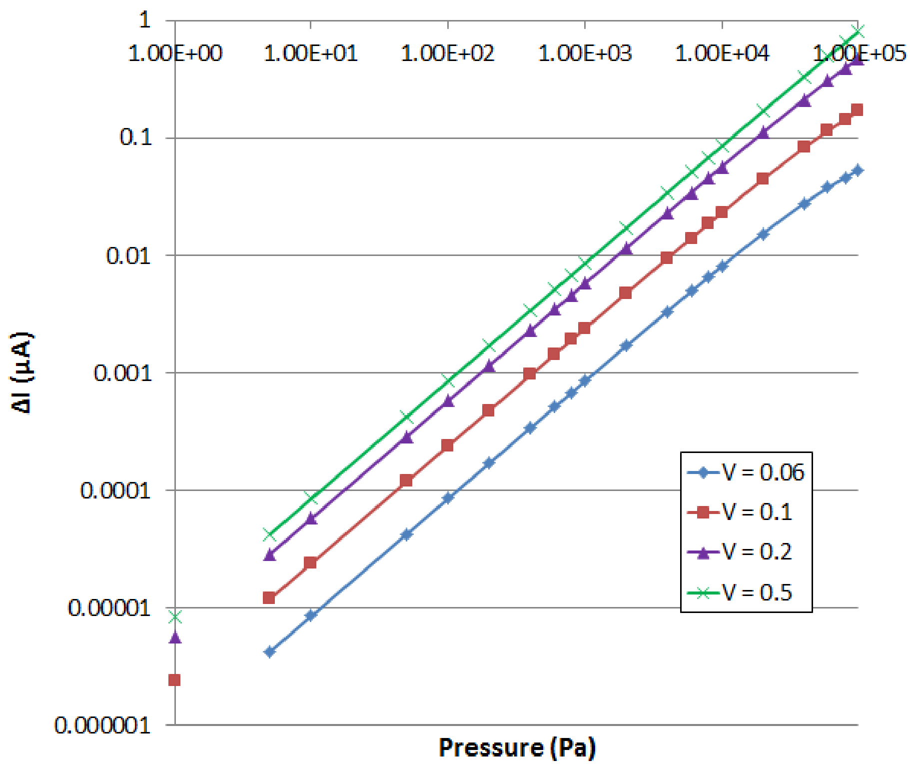


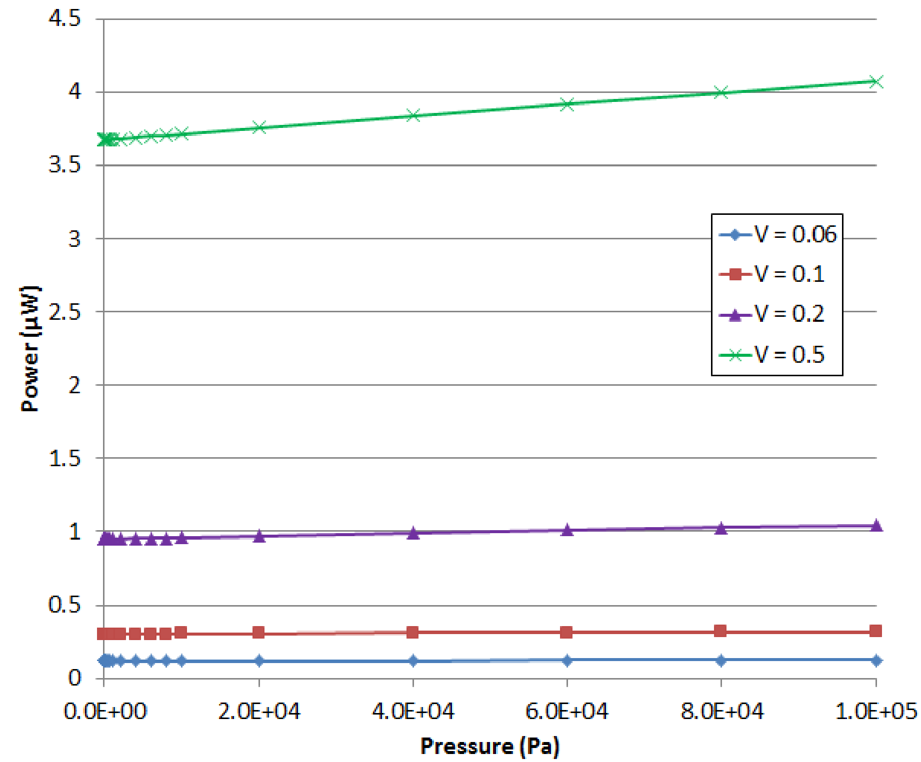
I vs P for 5 μm long suspended nanotube

Results

- Change in current compared to baseline value is linear:



ΔI vs P suspended nanotube

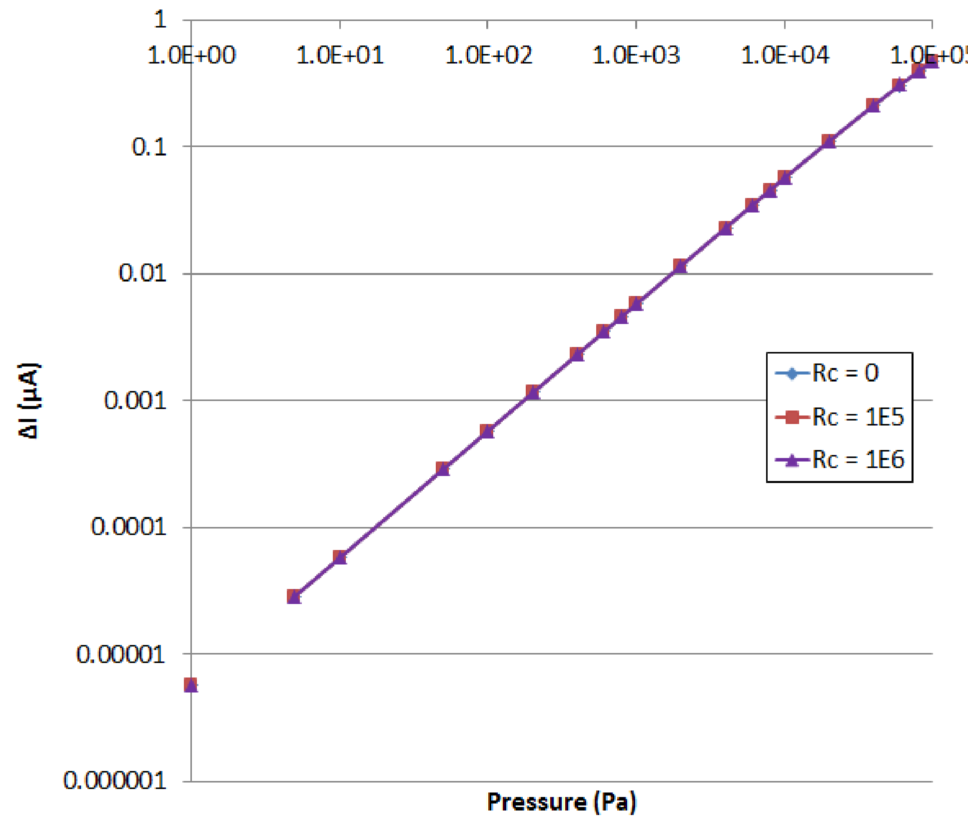


Power usage P suspended nanotube

- Increasing voltage increases sensitivity and range at the cost of power usage.

Results

- CNT based sensors have large range in contact resistance from substrate to device.
- A large thermal contact resistance may also be present.
- Contact resistance does not affect nanotube behavior, but complicates sensing.



ΔI vs P for 5 µm long suspended nanotube with different contact resistances

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Conclusions an Future Work

- Suspended nanotube behavior can be captured with 1-D model.
- Voltage vs. Current curve becomes non-linear due to changing resistance.
- Sensor design will be linear if current is the output over a range of pressures
- Currently looking at Platinum sensors, which can be fabricated in a more repeatable manner.

Acknowledgements

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- Linda del Castillo
- Sam Bae

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