Thermal transport & gas diffusion in CNT aerogels

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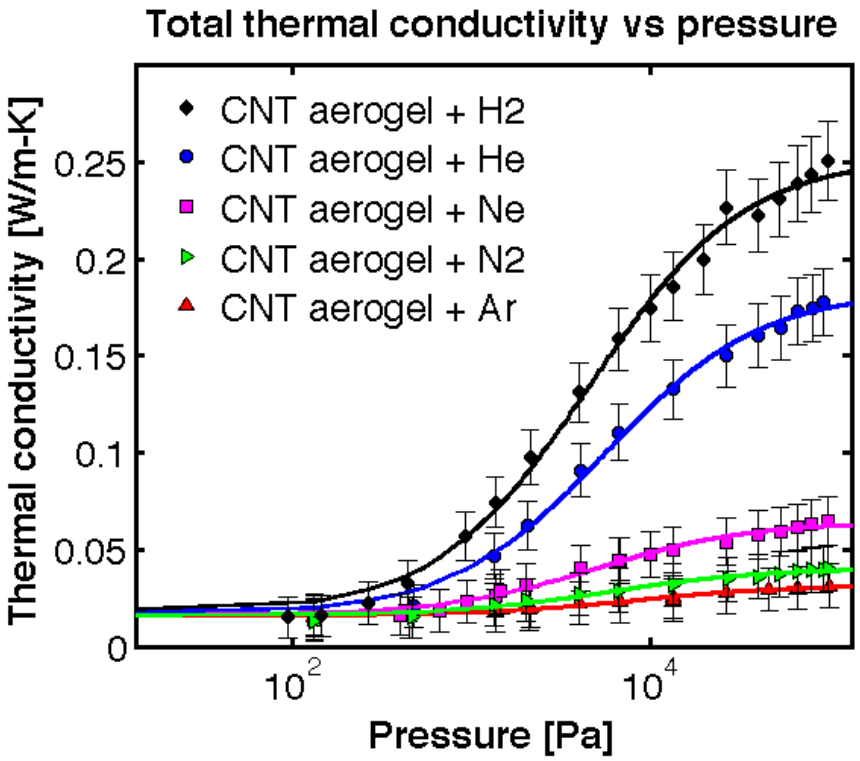
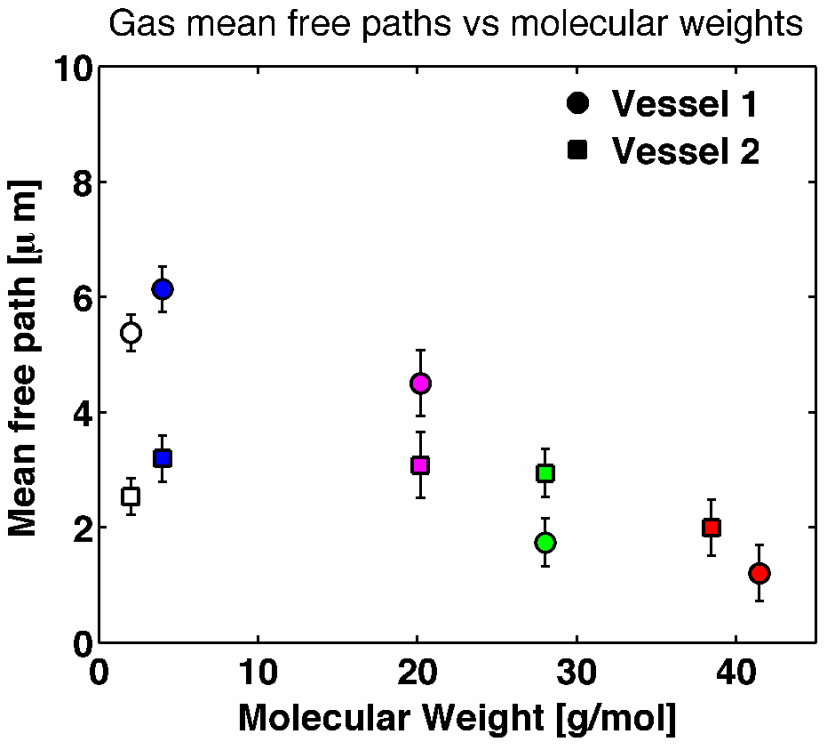
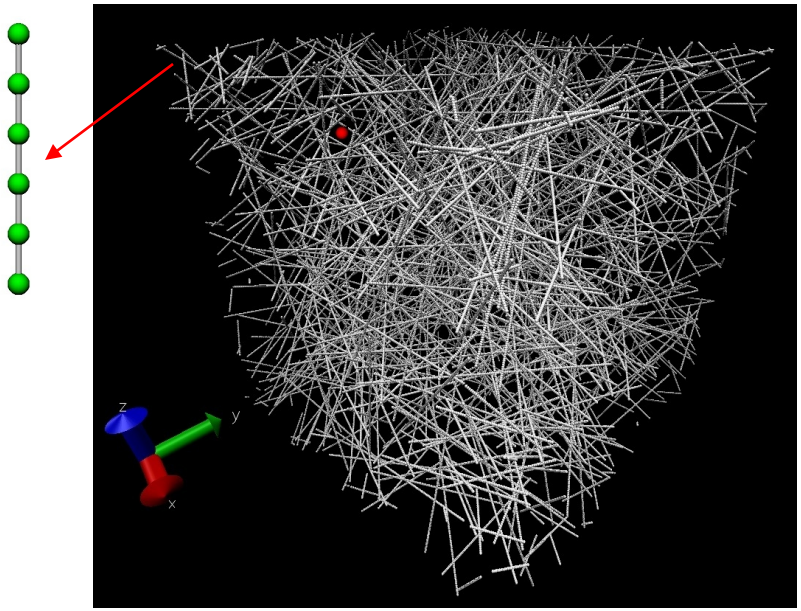
Background & Motivation

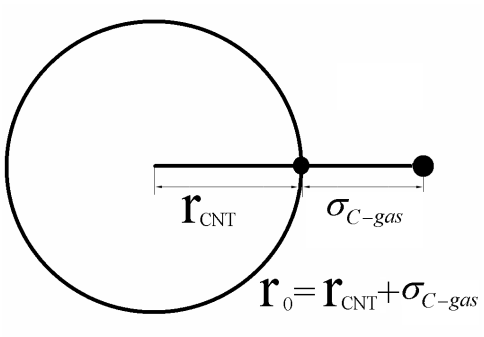




Gas mean free pass L_{KT} (2-7 um) >> Characteristic pore diameters d_c (2-50 nm)

Estimation of gas traveling distance in CNT aerogels



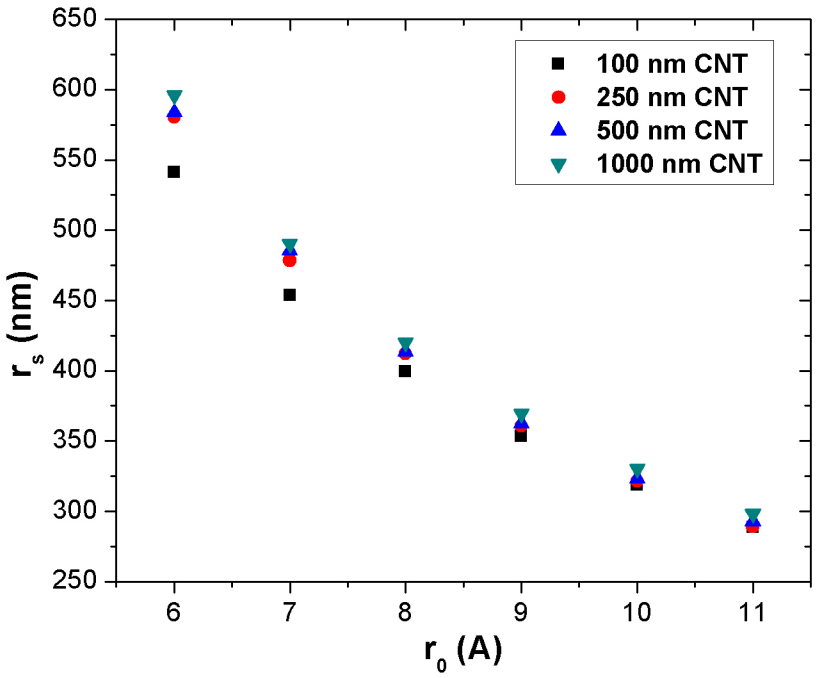


Procedure

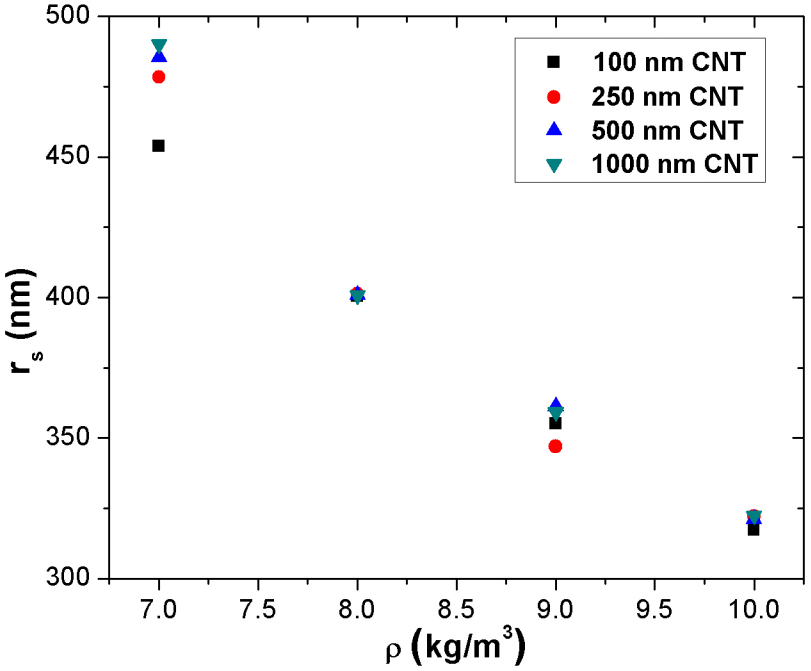
- Randomly choose a starting point and direction
- Move the gas atom 1A at the selected direction until collision happens
- Record the traveling distance
- Repeat the calculation 10,000 times
- Calculate the average gas traveling distance r_s

$r_s = L_{KT}$ or $r_s = d_c$???

Estimation of gas traveling distance in CNT aerogels



Traveling distance of different gas (radius) in CNT aerogels with density of 7 kg/m^3.



Traveling distance of Ne in CNT aerogels (different densities).

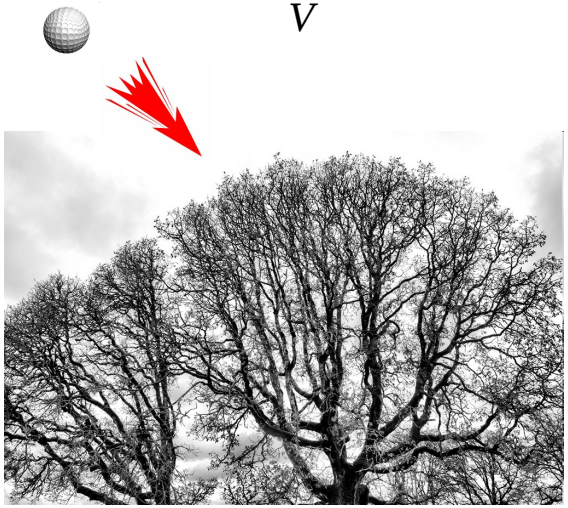
Ar (7.5A) – 450 nm **Ne (7.2A) – 470 nm** **He (6.5A) – 520 nm**

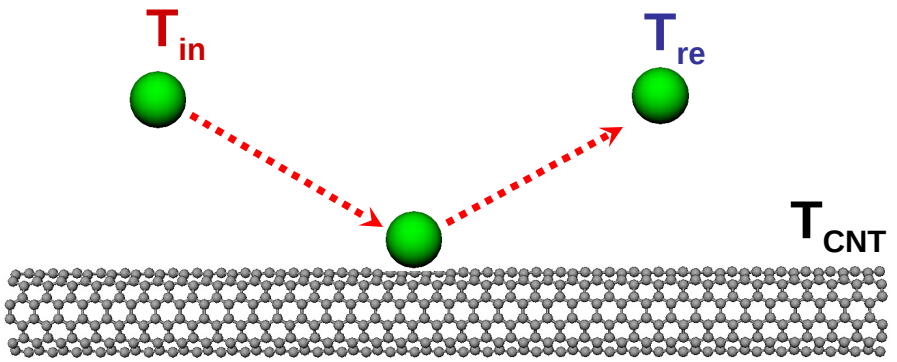
Experimental Measurements - Simulation

	Ar	Ne	He
Experiment (L_{KT})	2.7 um	5.6 um	6.6 um
Calculation (r_s)	450 nm	470 nm	520 nm

$$d_c << r_s < L_{KT}$$

$$\frac{V_{CNT}}{V} = 0.5\%$$





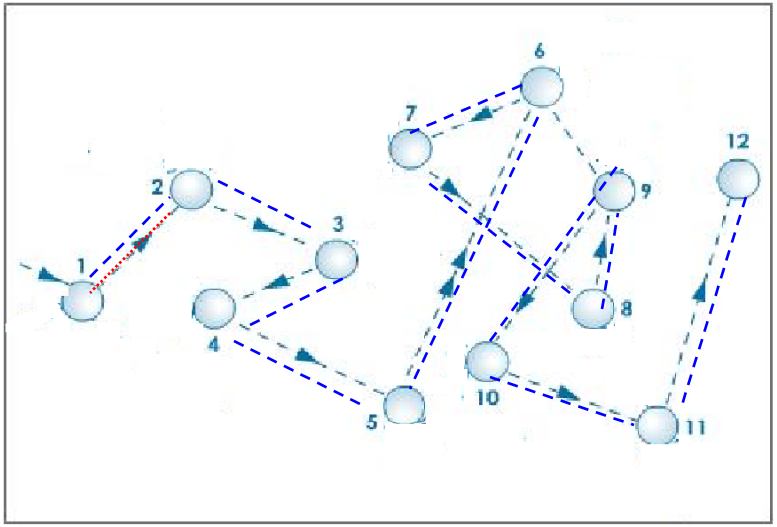
$T_{re} = T_{CNT}$???

Experimental Measurements - Simulation

$\alpha = \frac{E_{in} - E_{re}}{E_{in} - E_{w}}$ - thermal accommodation coefficient $\quad q = 1 - \alpha$

r_s - average gas traveling distance

r_e - average energy traveling distance



$$r_e = \alpha \times r_s + \alpha \times q \times 2r_s + \alpha \times q^2 \times 3r_s + \ldots + \alpha \times q^{n-1} \times n r_s$$

$$r_e = \{1 - q^n \times (1 + n - nq)\} \times \frac{r_s}{\alpha}$$

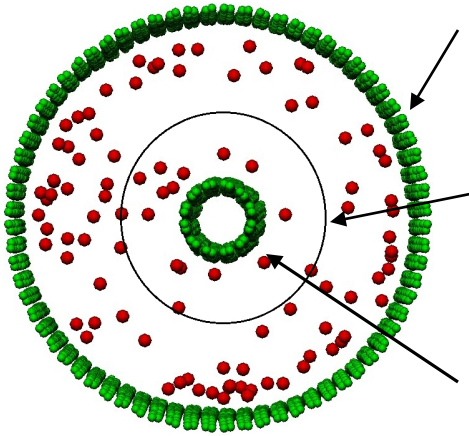
$0 < \alpha < 1$

$0 < q < 1$

$n \longrightarrow \infty$

$$\frac{r_e}{r_s} = \frac{1}{\alpha}$$

Thermal Accommodation Coefficient



T_{high}=320K

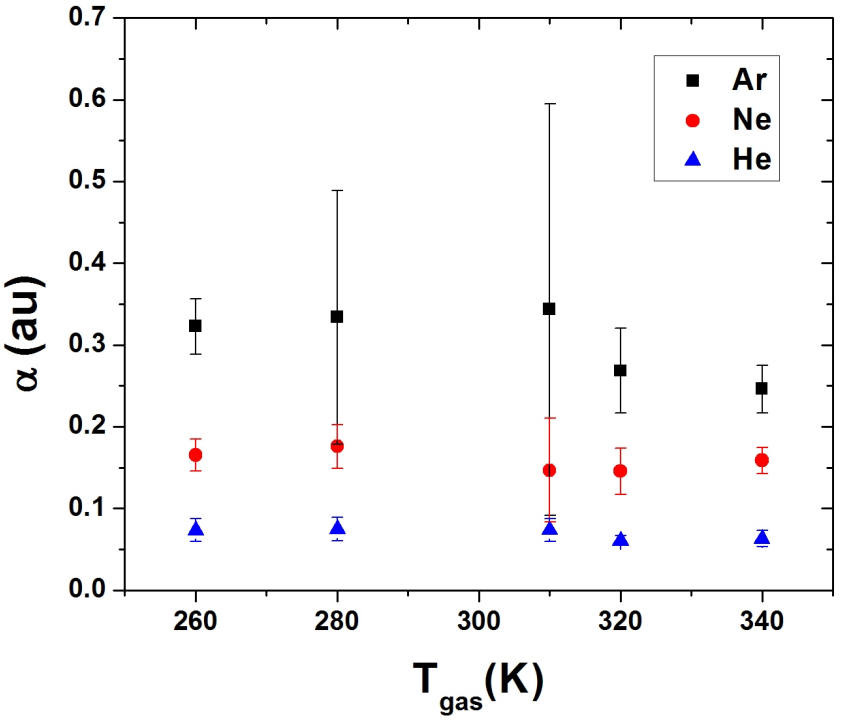
R_1=24 A

$R_3=R_2+R_{cut}$=13 A

T_{low}=300K

R_2=4 A

$$\alpha = \frac{E_{in} - E_{re}}{E_{in} - E_w}$$



NEMD simulation

CNT – AIREBO *CNT-gas – LJ potential*

N1 gas atoms go into the cylinder

N2 gas atoms go out from the cylinder

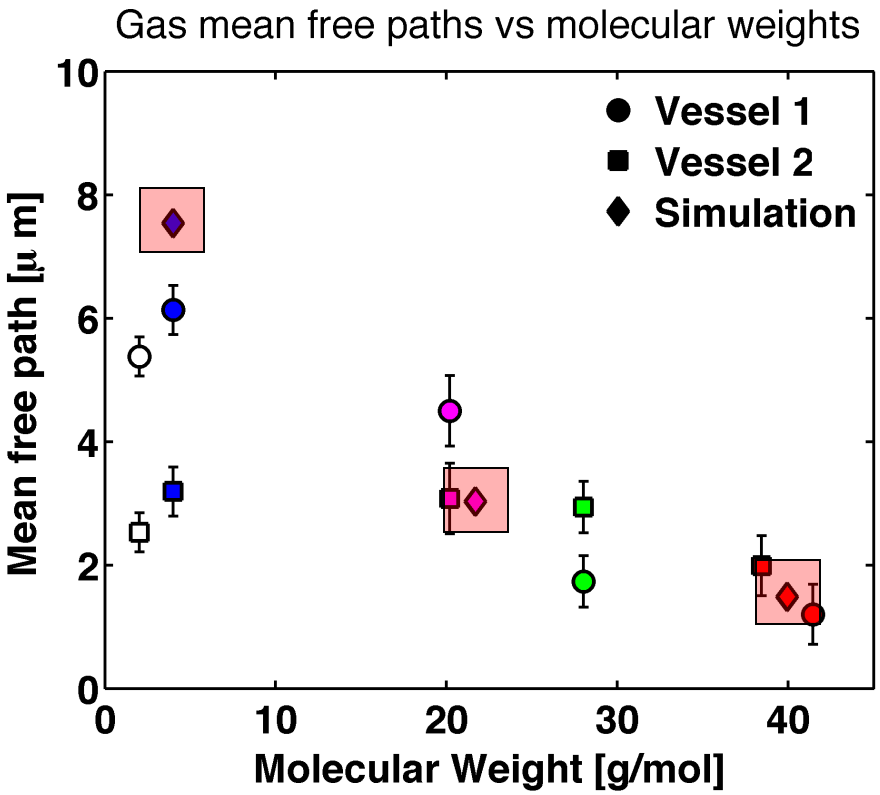
Record velocities (energy) of gas atoms

Experimental Measurements - Simulation

	Ar	Ne	He
r_s	450 nm	470 nm	520 nm
α	0.303	0.158	0.069

$$\frac{r_e}{r_s} = \frac{1}{\alpha}$$

	Ar	Ne	He
r_e	1.49um	3.03um	7.54um



$$r_e = L_{KT}$$

Summary

- Gas traveling distance in the CNT aerogel is calculated using the meso-scale CNT aerogel model.
- Gas-CNT thermal accommodation coefficient is calculated with NEMD simulations.
- Accommodation coefficient bridges the order-of-magnitude difference between the gas mean free path from experimental measurements and simulation.
- Mechanism of gas diffusion in CNT aerogel is proposed.

Thank You !