A Molecular Dynamics study on Ethanol/Water mixtures within Gold nanotubes of different sizes

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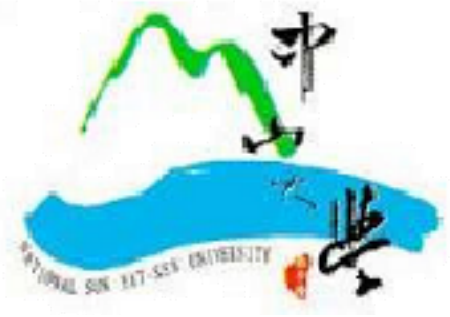
Outlines

- Material
- Simulation model
- Result and discussion
- Conclusion



Material

- Au nanotube
- Water molecules
- Ethanol molecules

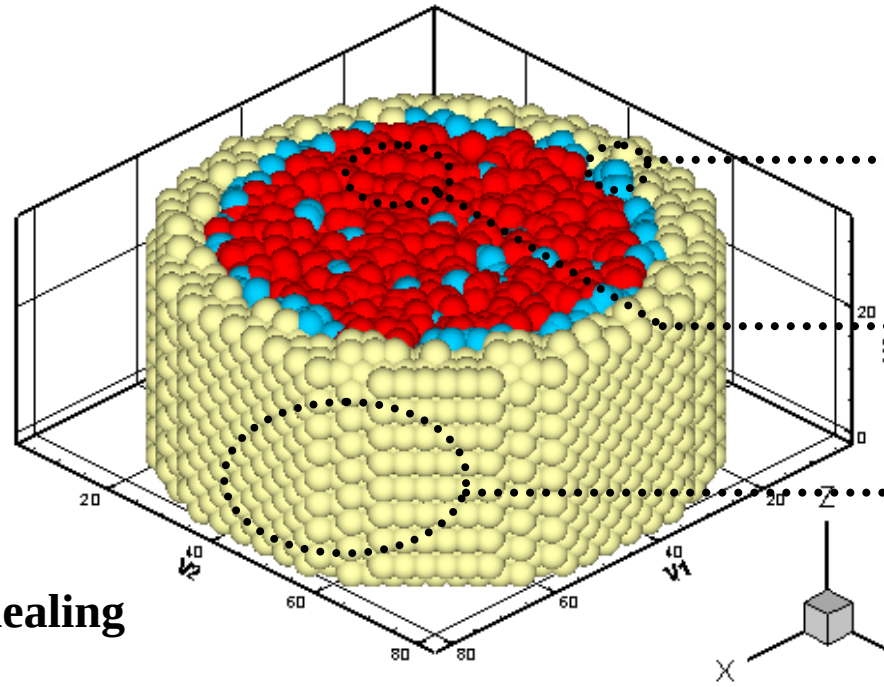
Simulation model

NVT system

300 K

Nose-Hoover

Simulation- Annealing



Blue bead
Water

Red bead
Ethanol

Yellow bead
Gold

Ethanol : water		25/75	50/50	75/25
N_{au}=2128 D =22.00 Å	E	153	288	405
	W	1173	735	345
N_{au}=2864 D =31.16 Å	E	306	576	810
	W	2346	1470	690

* The length of Z-direction is 32.632 Å in all cases.

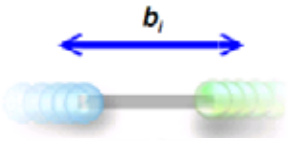
Simulation model

- **ENCAD**
  (water - water, water - ethanol, ethanol - ethanol)
- **Spohr**
  (water - Au)
- **Dreiding**
  (Au - ethanol)
- **Tight-Binding**
  (Au - Au)

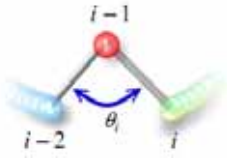
Simulation model

ENCAD (water-water, water-ethanol, ethanol-ethanol)

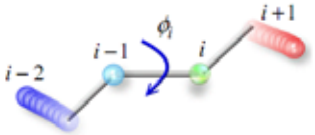
$$U_{tot} = U_{bond} + U_{bend} + U_{torsion} + U_{vdw} + U_{col}$$



$$U_{bond\ length} = \sum_{N=1}^{N_b} 1/2\ k_b^i\ (b_i - b_0^i)^2$$



$$U_{bending} = \sum_{N=1}^{N_\theta} 1/2\ k_\theta^i\ (\theta_i - \theta_0^i)^2$$



$$U_{dihedral} = \sum_{n=1}^{N_\varphi} K_\varphi^i\ \{1-\cos[\,n^i(\varphi_i - \varphi_0^i)]\}$$

$$U_{vdw} = [A_{SC}\varepsilon^{ij}(r_0^{ij}/r_{ij})^{12} - 2\varepsilon^{ij}(r_0^{ij}/r_{ij})^6 - S_{vdw}^A(r_{ij})]$$

$$U_{col} = 332 \sum_{\text{partial charges}} [q^i q^j / r_{ij} - S_{els}^A(r_{ij})]$$

Simulation model

Spohr (water - Au)

$$U_{M-H_2O} = U_{M-O}(r_{M-O}) + U_{M-H_1}(r_{M-H_1}) + U_{M-H_2}(r_{M-H_2})$$

$$U_{M-O}(r) = D_O[\exp(-2\beta_o(r - r_{e1})) - 2\exp(-\beta_o(r - r_{e1}))]$$

$$U_{M-H}(r) = \gamma D_0 \exp(-2\beta_H(r - r_{e2}))$$

Dreiding (Au - ethanol)

$$E_{ij} = D\left[\left(\frac{6}{Z-6}\right)\exp\left(Z\left(1-\frac{R_{ij}}{R}\right)\right) - \left(\frac{Z}{Z-6}\right)\left(\frac{R_{ij}}{R}\right)^{-6}\right]$$

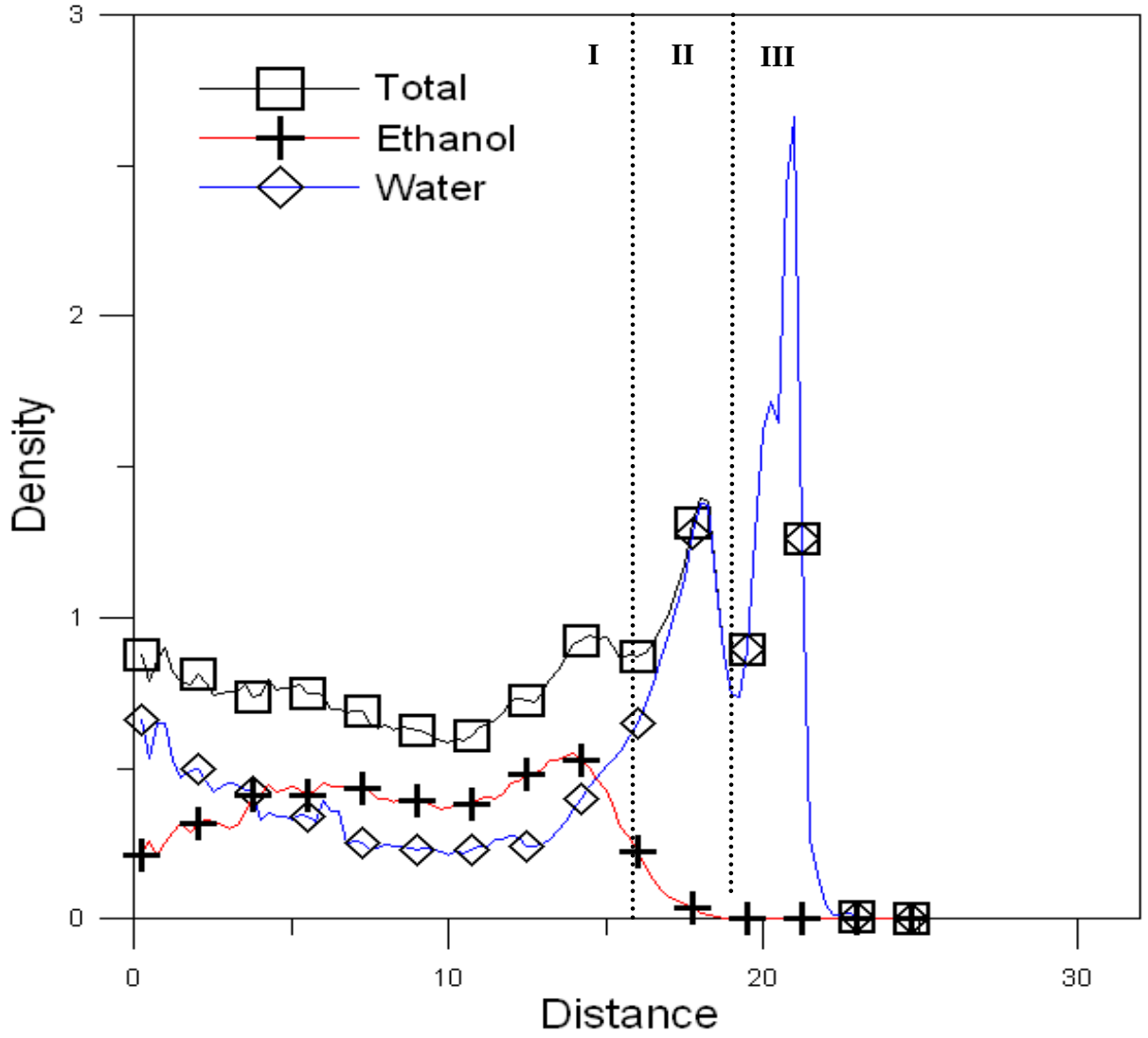
Tight-Binding (Au - Au)

$$E_c = \sum_i \left(E_B^i + E_R^i\right)$$

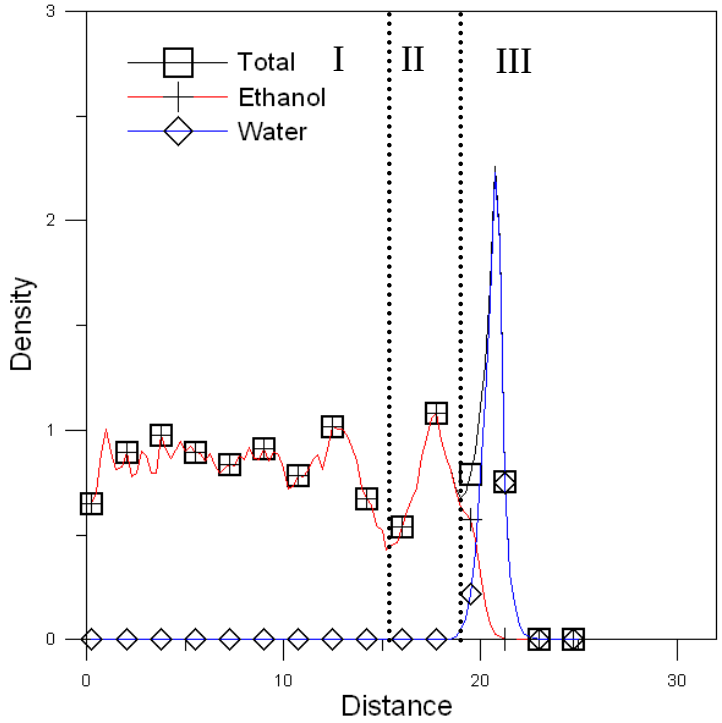
$$E_R^i = \sum_j A \cdot \exp\left\{-p\left(r_{ij}/r_0 - 1\right)\right\}$$

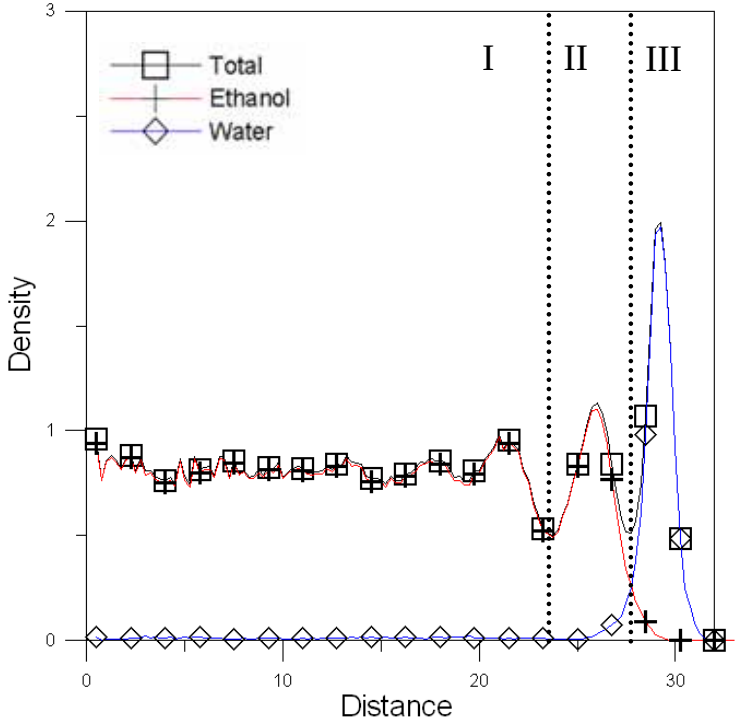
$$E_B^i = -\left\{\sum_j \xi^2 \cdot \exp\left[-2q\left(r_{ij}/r_0 - 1\right)\right]\right\}^{1/2}$$

Result and discussion

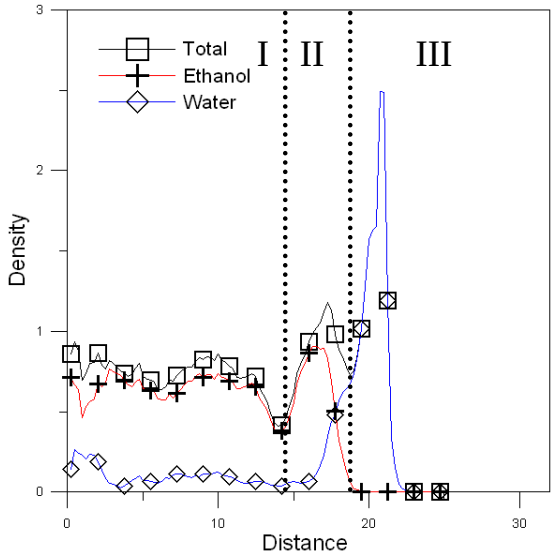


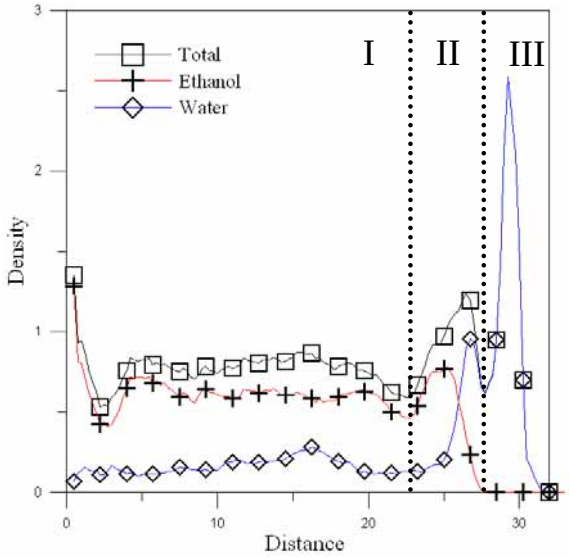
Result and discussion (W/E = 25/75)

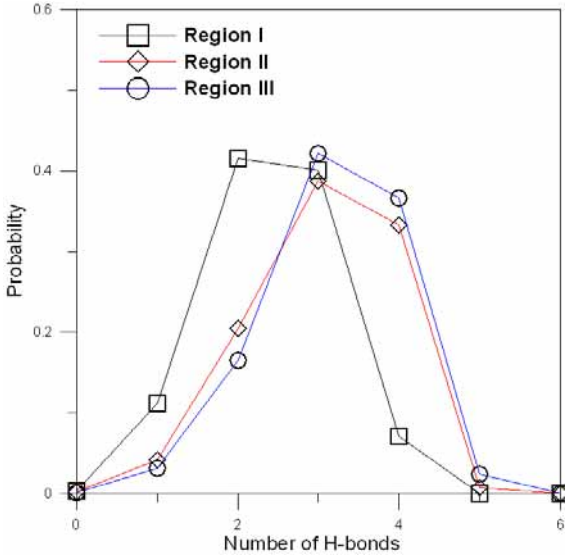


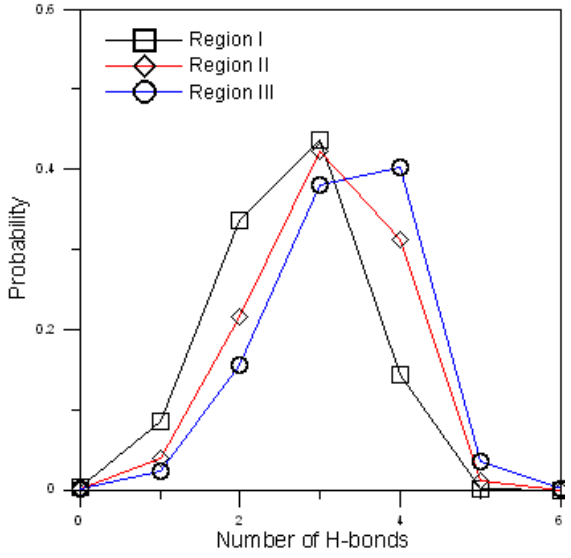


Result and discussion (W/E = 50/50)

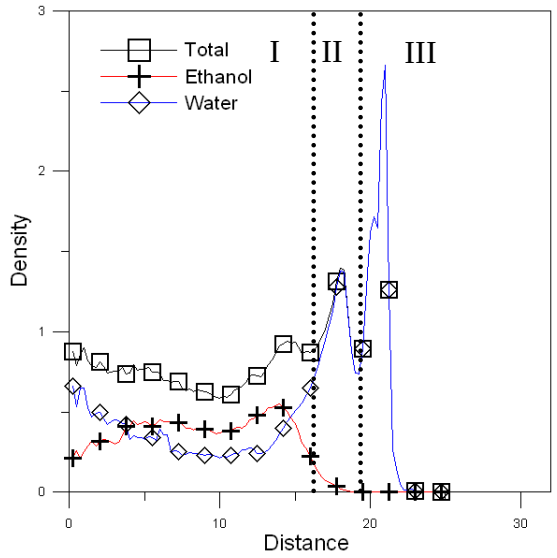


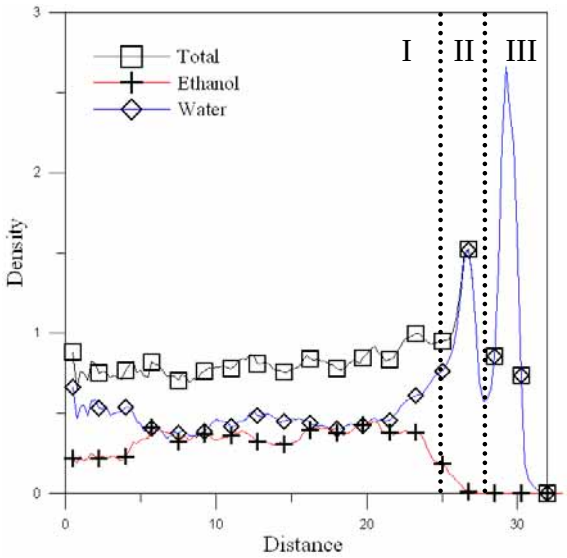


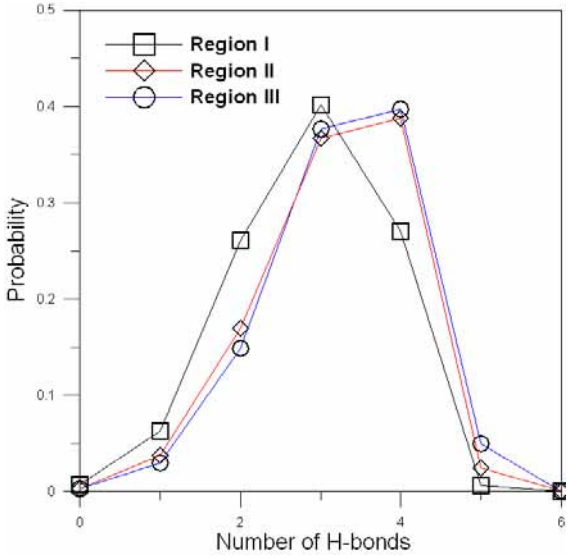


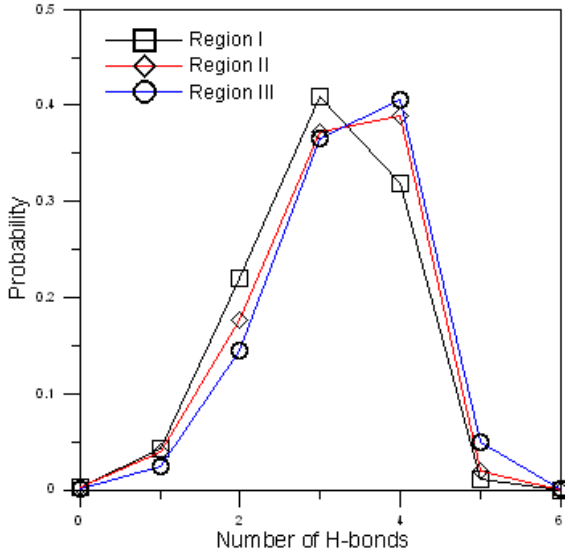


Result and discussion (W/E = 75/25)









Conclusion

- For the lower water weight fraction, there is no size effect.
- The water/ethanol weight fraction in Region I display a slight increase with the increase of Au nanotube diameter, indicating that if the diameter of Au nanotube is larger, the water/ethanol weight fraction in Region I will increase to the average weight fraction.

Thanks for your attending