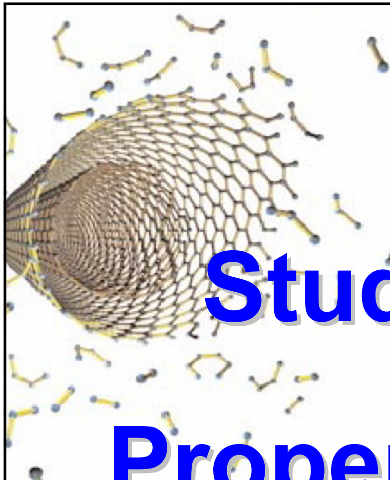

Study on Heat Conduction Properties of CNT Composites

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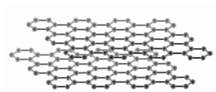
Shinshu University
Faculty of Engineering

Outline

- Introduction
- Computational models
- Numerical tools
- RVE including single straight CNT
- RVE including a curved CNT
- Study on CNT alignments
- Conclusions

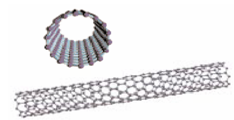
Introduction

➢Thermal conductivity of CNT (W/m·K)



Graphite
50~100

Diamond
3320



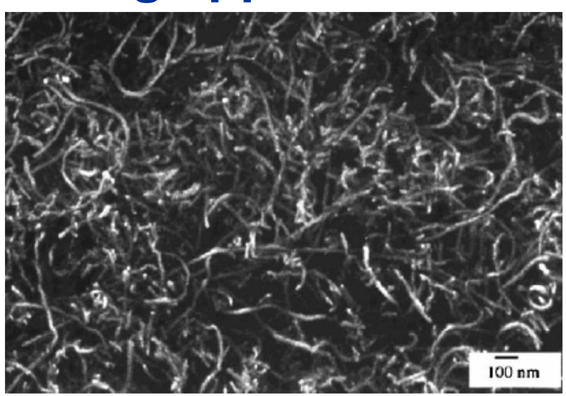
Nanotube
3000~6000

Resins: 0~1 W/m·K

Metals:

Fe	72	W/m·K
Al	240	W/m·K
Cu	390	W/m·K

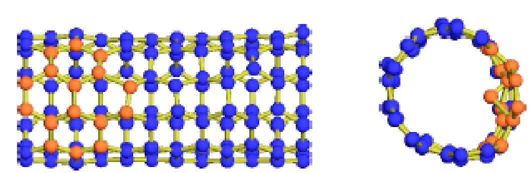
➢Promising applications



Nanotube-reinforced polymers

Computational Models

- Atomistic or molecular dynamics (MD) models



Classical MD: motion of molecules and atoms, governed by Hamilton's equation

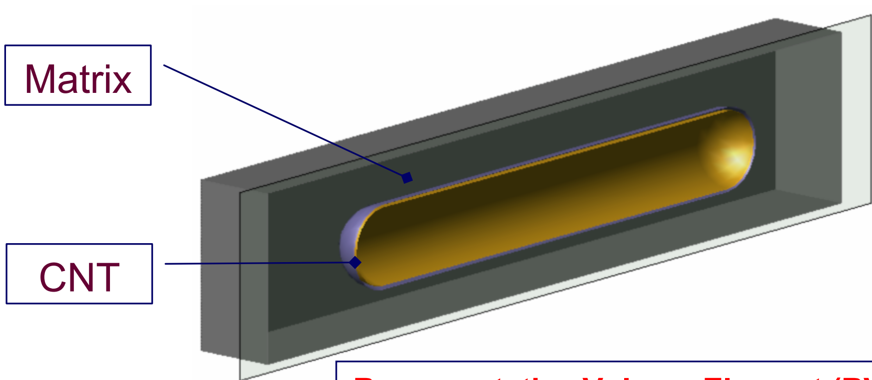
Ab initio: motion of electrons and nucleus, governed by Schrödinger's equation

Remarks:

- Limited to very small length and time scales;
- Suitable for only individual or isolated nanotubes, and cannot deal with CNT-based composites.

Computational Models (2)

◆ **Continuum approaches**



Representative Volume Element (RVE)

CNTs are treated as thin shells or solids in cylindrical shapes.

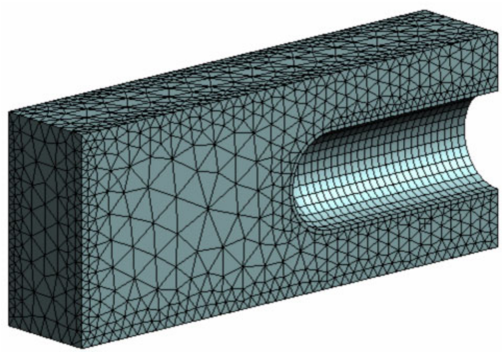
Their physical behavior is governed by continuum mechanics equations

Remarks:

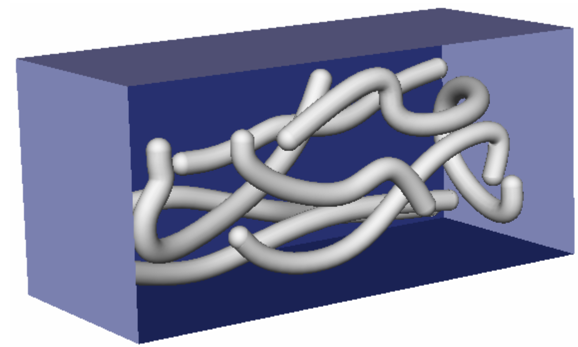
- **Capable of handling large length scale;**
- **Seems at present to be the only feasible approach for carrying some preliminary simulations of CNT-based composites.**

Numerical tools

◆ Mesh-based methods: FEM or BEM



FEM/BEM Mesh for a quarter of a unit model



An RVE including many curved CNTs

Remarks:

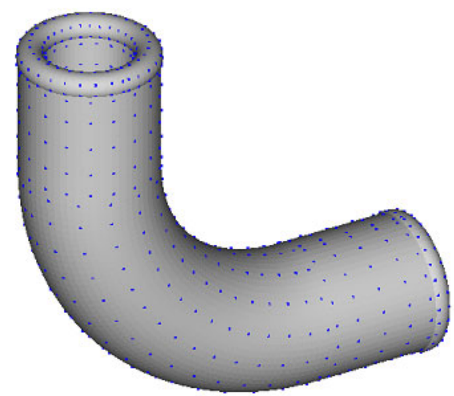
➢ When an RVE including many randomly scattered CNTs, the high quality finite/boundary elements are difficult and cumbersome to obtain.

Numerical tools (2)

◆ Hybrid Boundary Node Method (HBNM)

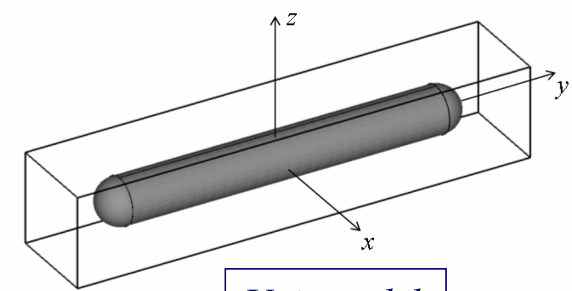
Main features:

- Combines a modified functional with the *Moving Least Squares* (MLS) approximation
- Boundary-only meshless method

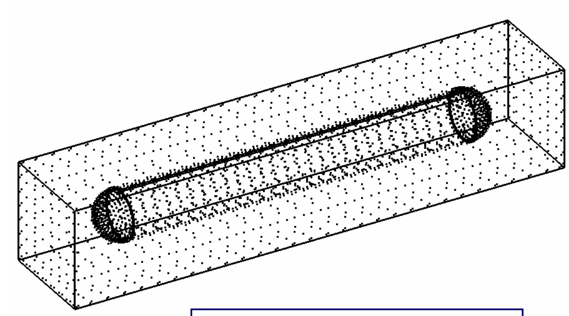


Example of meshless discretization

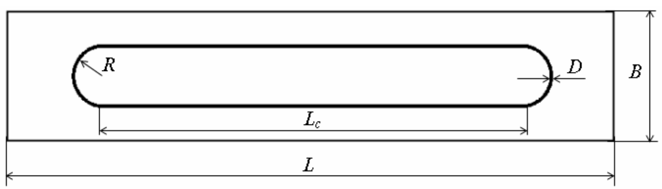
RVE with single (straight) CNT

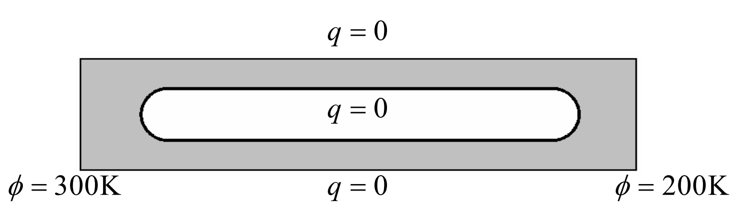


Unit model



Discretized model



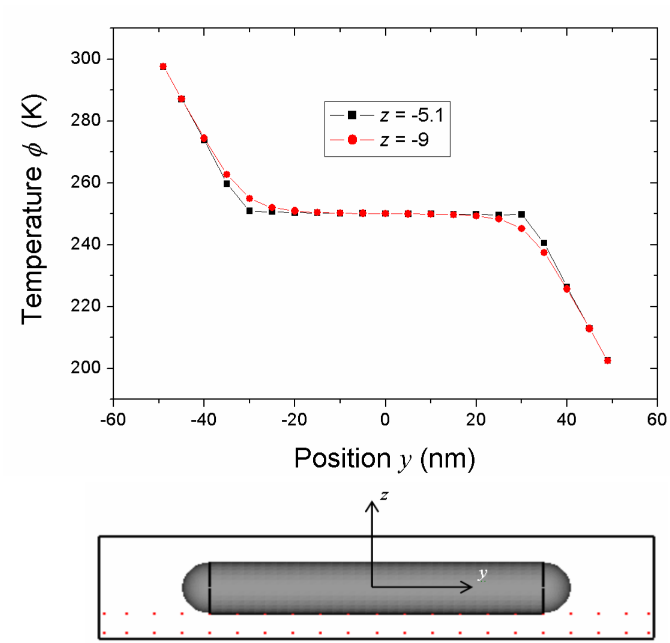


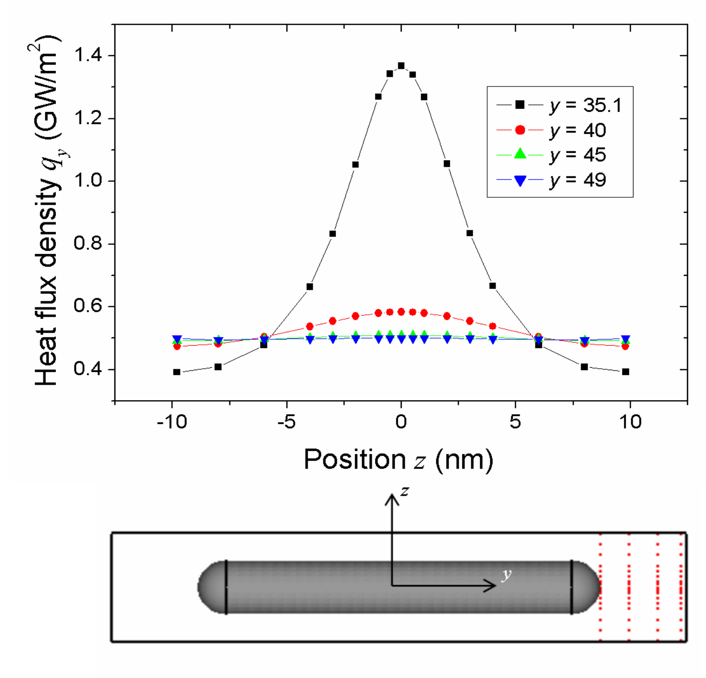
Boundary condition

B=20 nm, L=100 nm
L_c=70 nm, R=5 nm
D=0.4 nm

Heat conductivity:
Nanotube: 6000 W/m·K
Polymer: 0.19 W/m·K

RVE with single (straight) CNT (2)

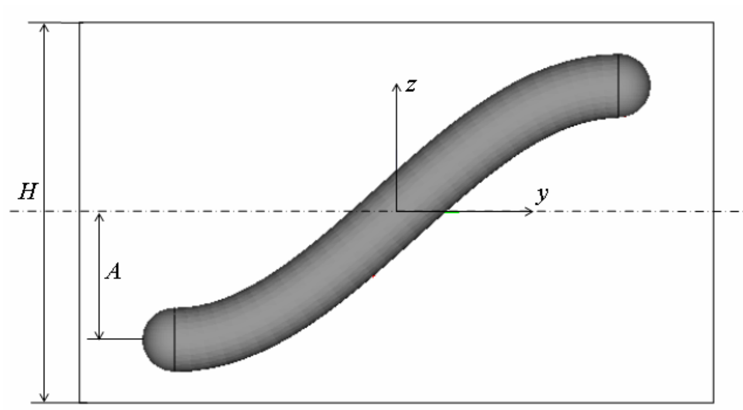


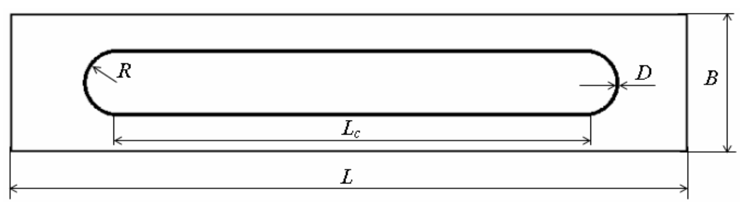


Volume fraction:	*15%*
Equivalent conductivity:	*0.6787* W/m·K (*3.57 times that of the polymer*)

RVE with single (curved) CNT

- **Dimensions and parameters**





$$z = A \sin\left(\frac{2\pi y}{L_c}\right)$$

H=60 nm, A=20 nm

L=100 nm, L_c=70 nm

R=5 nm, D=0.4 nm

B=20 nm

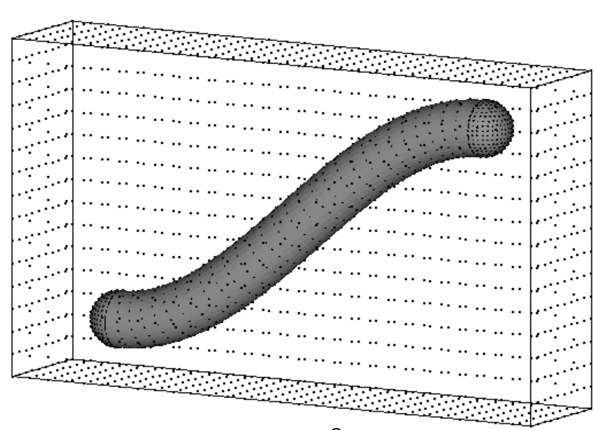
Conductivities

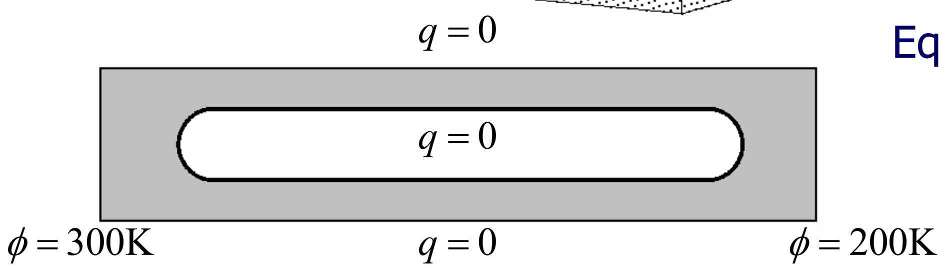
Nanotube: 6000 W/m·K

Polymer: 0.34 W/m·K

RVE with single (curved) CNT (2)

- **Discretization and boundary conditions**





Polymer matrix: 2984 nodes

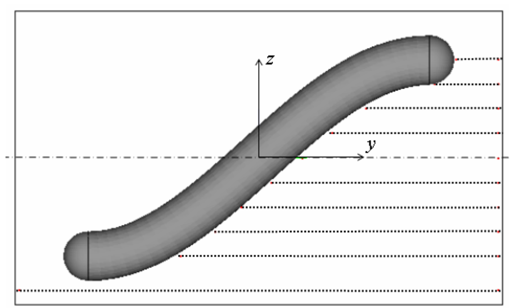
Carbon nanotube: 2208 nodes

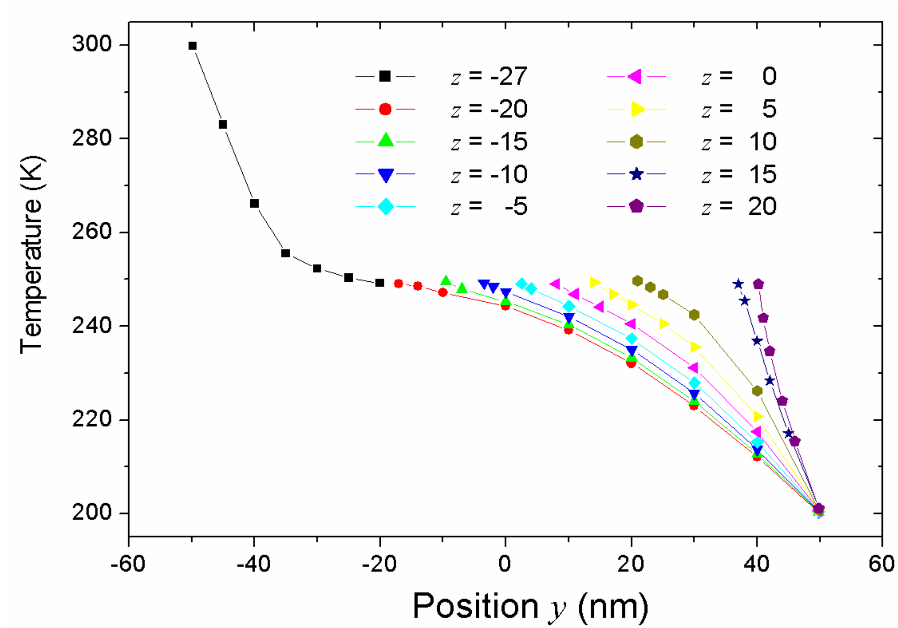
Equivalent heat conductivity

$$\kappa = -\frac{qL}{\Delta\phi}$$

RVE with single (curved) CNT (3)

- **Temperature distribution**





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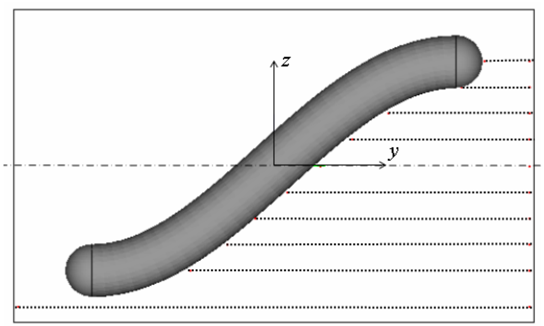
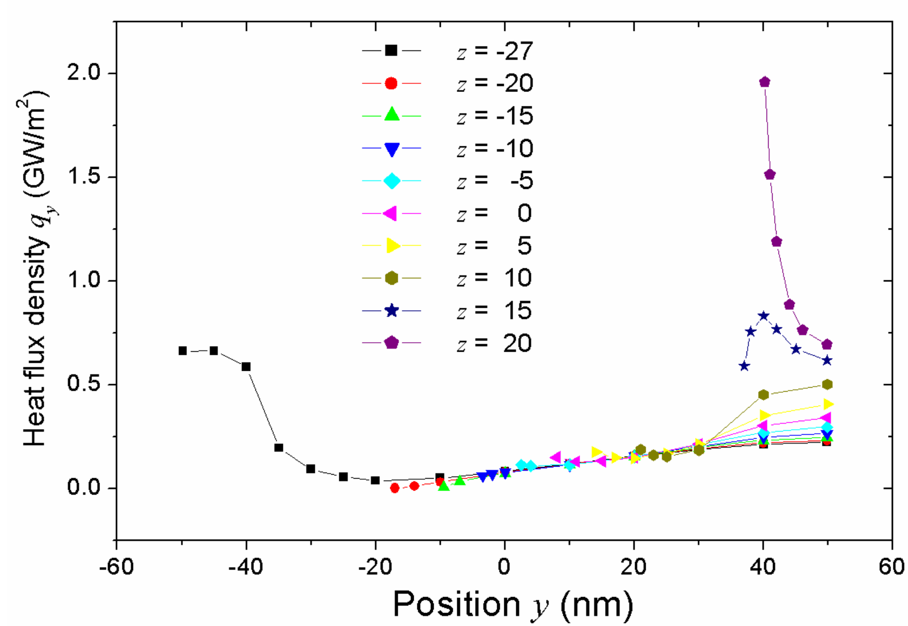
RVE with single (curved) CNT (4)

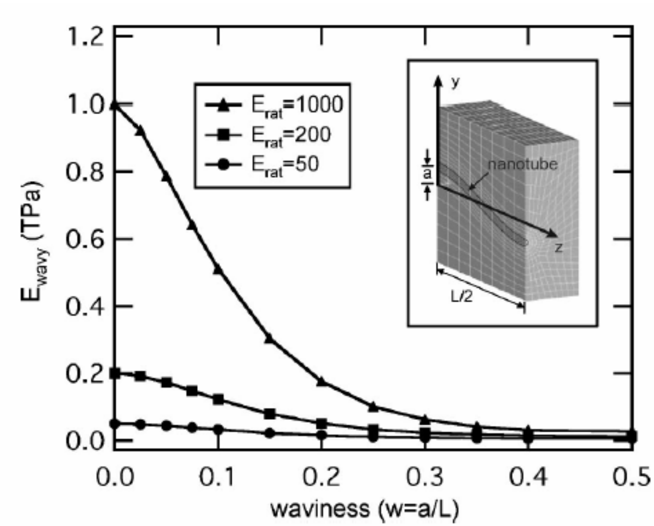
- **Flux distribution**



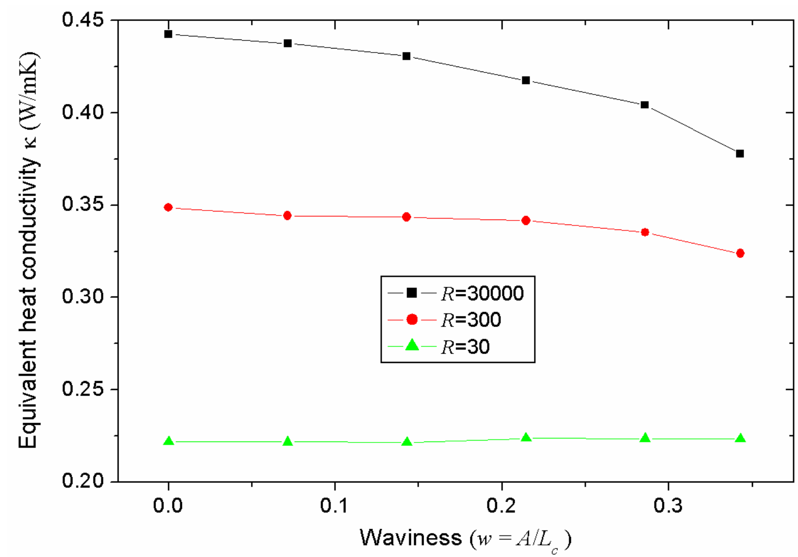


RVE with single (curved) CNT (5)

- **Impact of CNT curvature on equivalent properties**

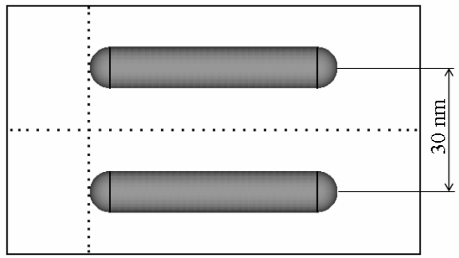


Results for elasticity problem
Appl. Phys. Lett. (2002)

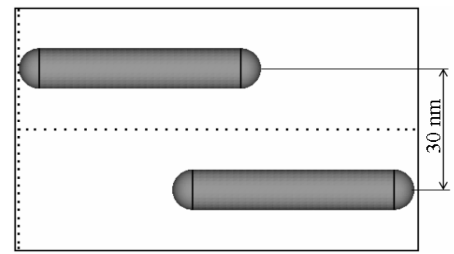


Results for heat conduction problem

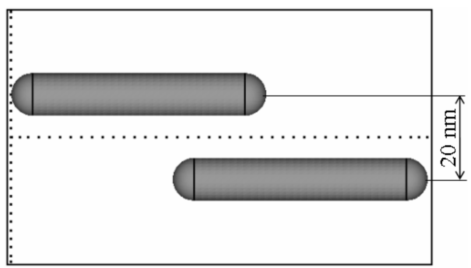
Study on CNT alignments



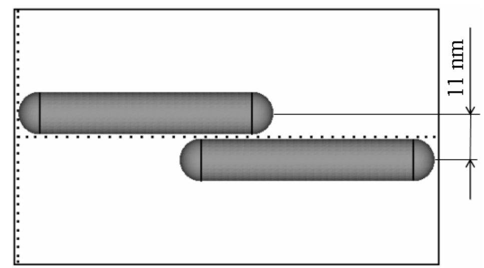
(a)



(b)



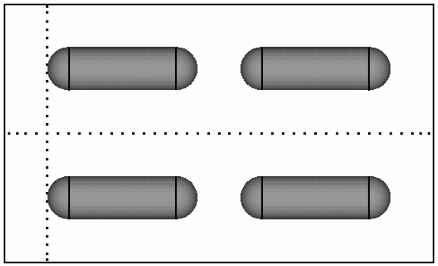
(c)

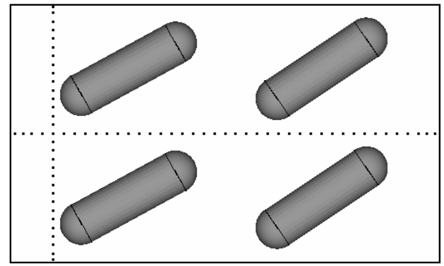


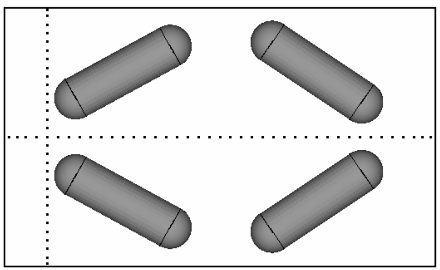
(d)

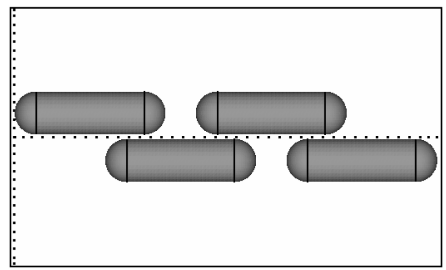
CNT alignments	(a)	(b)	(c)	(d)
Conductivity (W/m·K)	0.7160	1.005	1.124	1.441

Study on CNT alignments (2)


(a)


(b)


(c)


(d)

CNT alignments	(a)	(b)	(c)	(d)
Conductivity (W/m·K)	0.6974	0.5993	0.6015	0.9736

Conclusions

- The HBNM has been successfully applied to heat conduction analysis of CNT-based composites
- Insight into heat conduction behavior gained:
  - temperature distribution within the CNT is almost uniform
  - heat flux concentration occurs at the tips of the CNT
  - equivalent heat conductivity is less affected by the curvature of the CNT (unlike Young modulus)
  - dispersion of CNTs has a strong influence on the thermal properties of the nano-composites
- The HBNM combined with FMM should be capable of solving an RVE containing many randomly distributed CNTs