

# **An Application of the meshless BEM to Evaluation of the Thermal Properties of CNT Composites**

**Masa. Tanaka, J. Zhang, T. Matsumoto**

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Shinshu University  
Faculty of Engineering





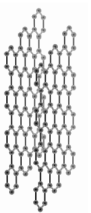
# Outline

- Introduction
- HBNM for single domain
- Multi-domain HBNM
- Modeling of RVE with single CNT
- Numerical results
- Conclusions

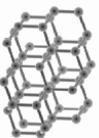


# Introduction

## ➤ Thermal conductivity of CNT (W/mK)



**Graphite**  
**50~100**



**Diamond**  
**3320**



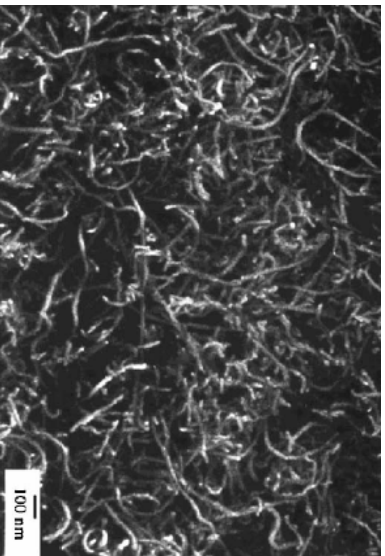
**Nanotube**  
**3000~6000**

**Resins: 0~1 W/mK**

**Metals:**

|           |            |             |
|-----------|------------|-------------|
| <b>Fe</b> | <b>72</b>  | <b>W/mK</b> |
| <b>Al</b> | <b>240</b> | <b>W/mK</b> |
| <b>Cu</b> | <b>390</b> | <b>W/mK</b> |

## ➤ Promising applications



**Nanotube-reinforced polymers**



# HBNM for single domain

- By combining a modified functional with the *Moving Least Squares* (MLS) approximation, the HBNM is a boundary-only truly meshless method
- Three independent variables
  - internal temperature

$$\phi = \sum_{I=1}^N \phi_I^s x_I$$

$$\phi_I^s = \frac{1}{\kappa} \frac{1}{4\pi r^3(Q, \mathbf{s}_I)}$$

- Boundary temperature and normal flux

$$\tilde{\phi}(\mathbf{s}) = \sum_{I=1}^N \Phi_I(\mathbf{s}) \hat{\phi}_I$$

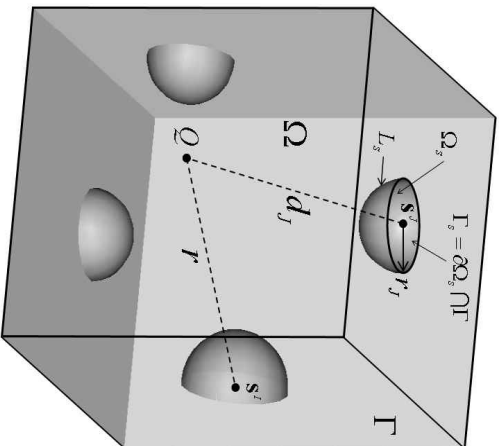
$$\tilde{q}(\mathbf{s}) = \sum_{I=1}^N \Phi_I(\mathbf{s}) \hat{q}_I$$



# HBNMM for single domain (2)

## ➤ Local weak form

$$\int_{\Gamma} (q - \tilde{q}) \delta \phi d\Gamma - \int_{\Omega} \phi_{,ii} \delta \phi d\Omega + \int_{\Gamma_q} (\tilde{q} - \bar{q}) \delta \tilde{\phi} d\Gamma - \int_{\Gamma} (\phi - \tilde{\phi}) \delta \tilde{q} d\Gamma = 0$$



$$\sum_{I=1}^n \int_{\Gamma_s} \frac{\partial \phi_I^s}{\partial n} \nu_j(Q) x_j d\Gamma = \sum_{I=1}^n \int_{\Gamma_s} \Phi_I(\mathbf{s}) \nu_j(Q) \hat{q}_I d\Gamma$$

$$\sum_{I=1}^n \int_{\Gamma_s} \phi_I^s \nu_j(Q) x_j d\Gamma = \sum_{I=1}^n \int_{\Gamma_s} \Phi_I(\mathbf{s}) \nu_j(Q) \hat{\phi}_I d\Gamma$$



# HBNMM for single domain (3)

➤ System of equations – final form

$$\mathbf{U}\mathbf{x} = \mathbf{H}\hat{\mathbf{q}}$$

$$\mathbf{V}\mathbf{x} = \mathbf{H}\hat{\boldsymbol{\phi}}$$

where

$$U_{IJ} = \int_{\Gamma'_I} \frac{\partial \phi_I^s}{\partial n} \nu_J(\mathcal{Q}) d\Gamma$$

$$V_{IJ} = \int_{\Gamma'_I} \phi_I^s \nu_J(\mathcal{Q}) d\Gamma$$

$$H_{IJ} = \int_{\Gamma'_I} \Phi_I(\mathbf{s}) \nu_J(\mathcal{Q}) d\Gamma$$

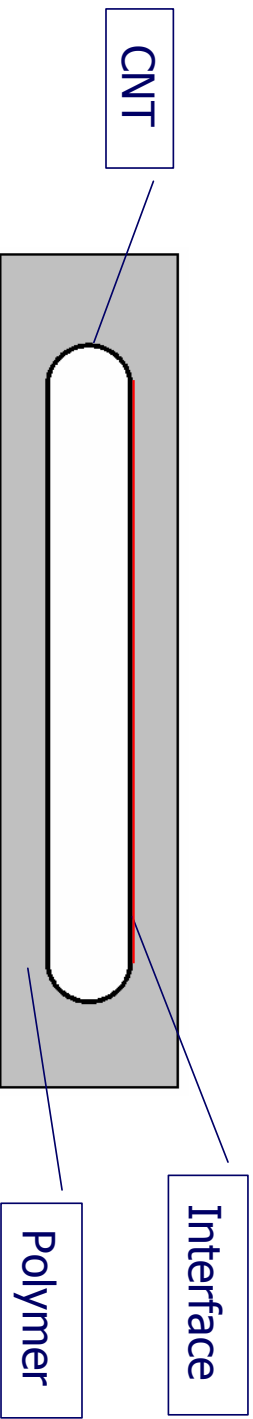


# Multi-domain HBNM

- CNT and Polymer

$$\begin{bmatrix} U_{00}^P & U_{01}^P \\ U_{10}^P & U_{11}^P \end{bmatrix} \begin{Bmatrix} x_0^P \\ x_1^P \end{Bmatrix} = \begin{Bmatrix} H_0^P \hat{\phi}_0^P \\ H_1^P \hat{\phi}_1^P \end{Bmatrix} \quad \begin{bmatrix} V_{00}^P & V_{01}^P \\ V_{10}^P & V_{11}^P \end{bmatrix} \begin{Bmatrix} x_0^P \\ x_1^P \end{Bmatrix} = \begin{Bmatrix} H_0^P \hat{q}_0^P \\ H_1^P \hat{q}_1^P \end{Bmatrix}$$

$$\begin{bmatrix} U_{00}^n & U_{01}^n \\ U_{10}^n & U_{11}^n \end{bmatrix} \begin{Bmatrix} x_0^n \\ x_1^n \end{Bmatrix} = \begin{Bmatrix} H_0^n \hat{\phi}_0^n \\ H_1^n \hat{\phi}_1^n \end{Bmatrix} \quad \begin{bmatrix} V_{00}^n & V_{01}^n \\ V_{10}^n & V_{11}^n \end{bmatrix} \begin{Bmatrix} x_0^n \\ x_1^n \end{Bmatrix} = \begin{Bmatrix} H_0^n \hat{q}_0^n \\ H_1^n \hat{q}_1^n \end{Bmatrix}$$





# Multi-domain HBNNM (2)

- Continuity and equilibrium at the interface

$$\left\{ \phi_1^p \right\} = \left\{ \phi_1^n \right\} \quad \left\{ q_1^p \right\} = - \left\{ q_1^n \right\}$$

- Assembled system of equations

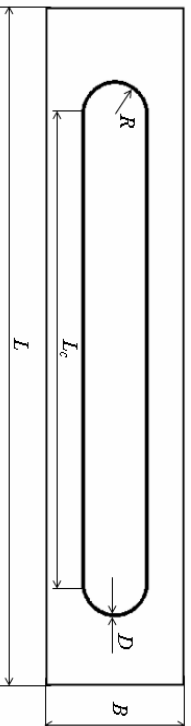
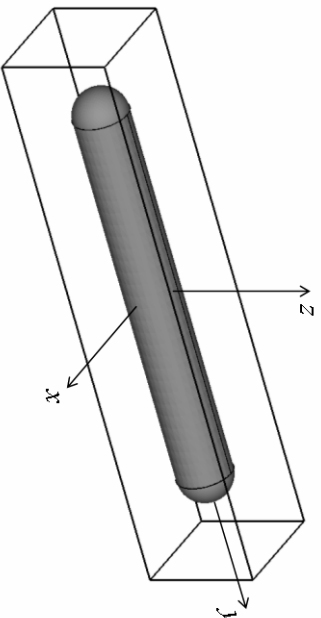
$$\begin{bmatrix} A_{00}^p & A_{01}^p & 0 & 0 \\ U_{10}^p & U_{11}^p & -U_{10}^n & -U_{11}^n \\ V_{10}^p & V_{11}^p & V_{10}^n & V_{11}^n \\ 0 & 0 & A_{00}^n & A_{01}^n \end{bmatrix} \begin{Bmatrix} x_0^p \\ x_1^p \\ x_0^n \\ x_1^n \end{Bmatrix} = \begin{Bmatrix} H_0^p d_0^p \\ 0 \\ 0 \\ H_0^n d_0^n \end{Bmatrix}$$





# RVE with single CNT

- Dimensions and parameters



$B=20$  nm,  $L=100$  nm

$L_c=70$  nm,  $R=5$  nm

$D=0.4$  nm

Conductivities

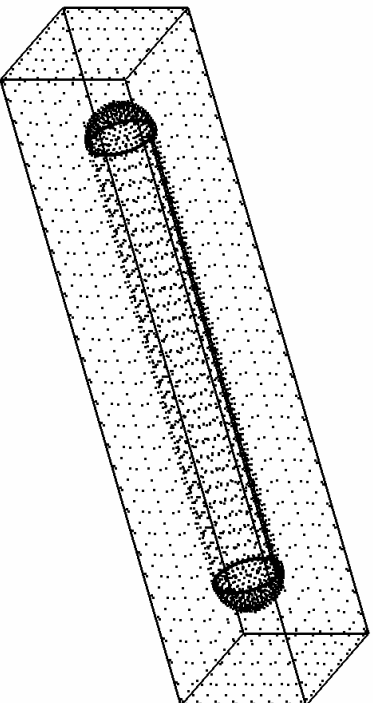
Nanotube:  $6000$  W/m·K

Polymer:  $0.19$  W/m·K



# RVE with single CNT (2)

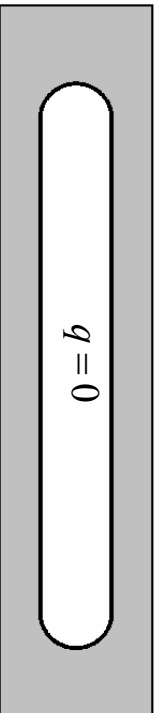
- Discretization and boundary conditions



Polymer matrix: 2192 nodes

Carbon nanotube: 2208 nodes

$q = 0$



$\phi = 300\text{K}$

$q = 0$

$\phi = 200\text{K}$

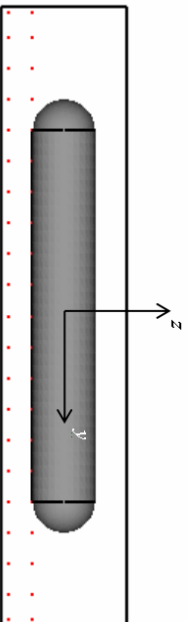
Equivalent heat conductivity

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



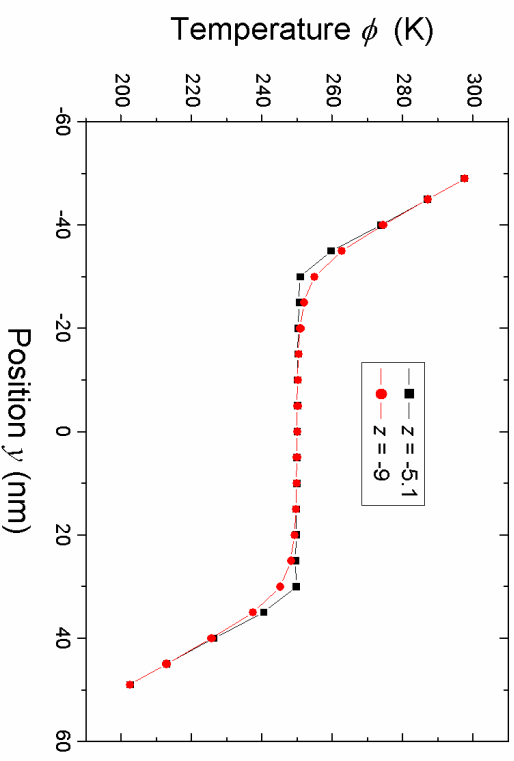
# Results

## Temperature distribution



Volume fraction:  
15%

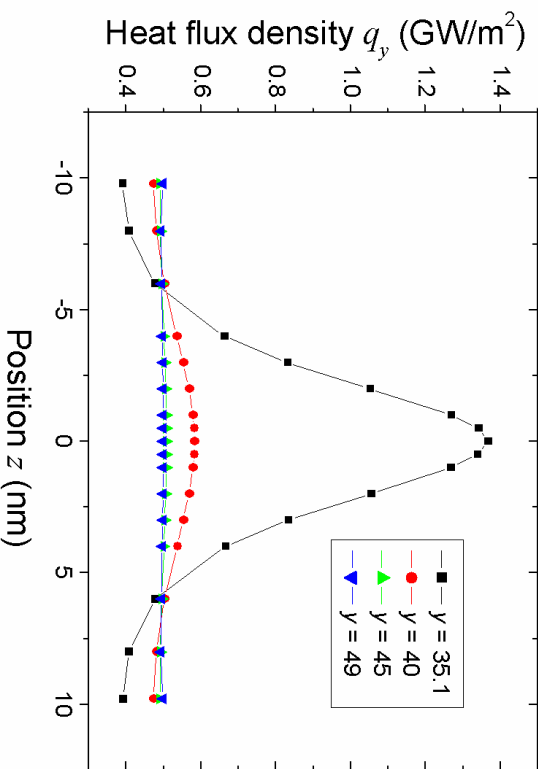
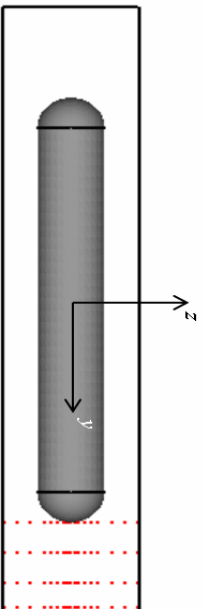
Equivalent conductivity:  
0.6787 W/m·K  
(3.57 times that of the matrix)





# Results (2)

- Flux distribution



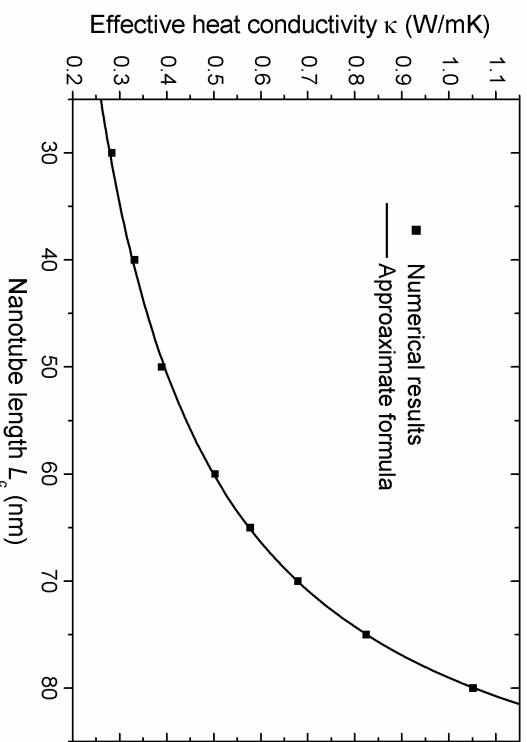


# Results (3)

- Equivalent heat conductivity as a function of CNT length

$$\kappa^e = \kappa^m \frac{L}{L - L_c - 0.4R}$$

Approximate formula





# 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