Evaluation of heat conducting properties of curved-CNT composites by the hybrid BNM

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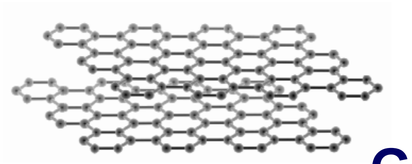
Outline

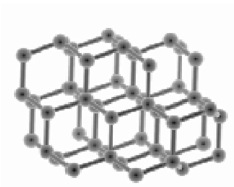
- Introduction
- HBNM for single domain
- Multi-domain HBNM
- Modeling of RVE with curved CNT
- Numerical results
- Conclusions

Introduction

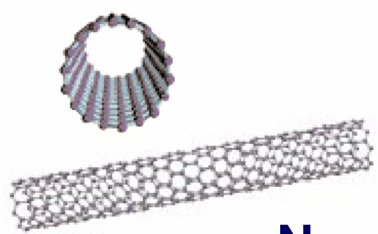
➢ Thermal properties of CNT



Graphite 50~100 W/mK



Diamond 3320 W/mK



Nanotube 3000~6000 W/mK

Resin 0~1 W/mK

Fe 72 W/mK

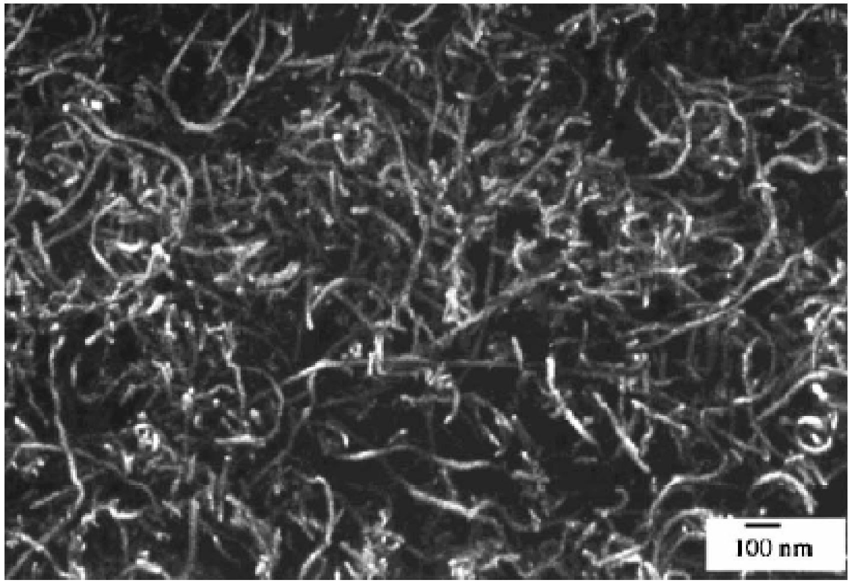
Al 240 W/mK

Cu 390 W/mK

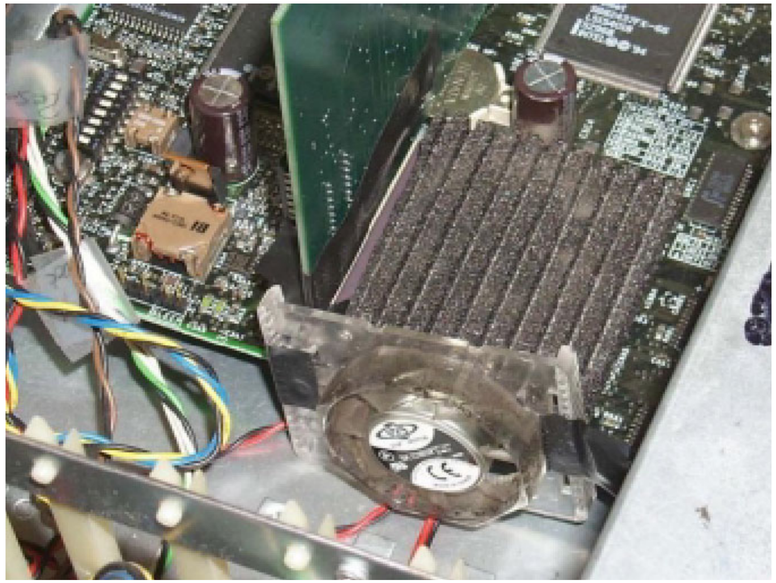
Background (1)

- **Promising applications**

Nanotube-reinforced polymers

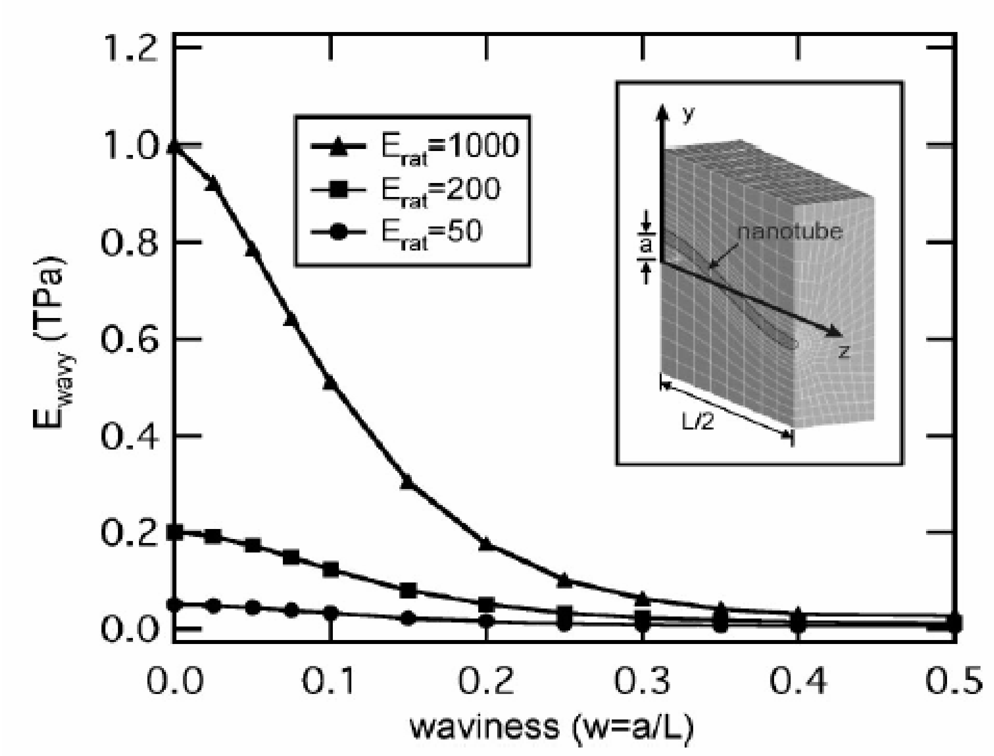


High-performance heat transport management



Background (2)

- **Effects of CNT curvature on properties**

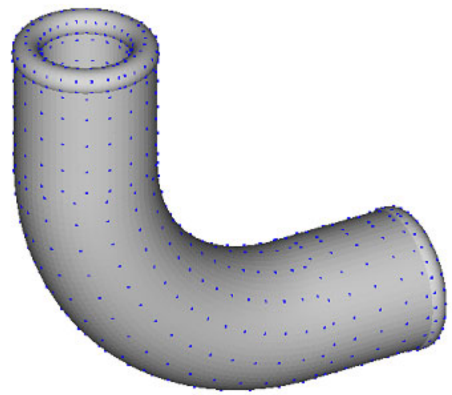


The equivalent Young's modulus quickly decreases with increasing nanotube curvature

HBNM for single domain

Main features:

- Combines modified functional with the *Moving Least Squares* (MLS) approximation
- Boundary-only truly meshless method
- Three independent variables
  - internal temperature ϕ
  - boundary temperature $\tilde{\phi}$
  - boundary normal flux $\tilde{q}$



Example of meshless discretization

HBNM for single domain (2)

➢ Variables approximation

- Domain variables

$$\phi = \sum_{I=1}^{N} \phi_I^s x_I \qquad \phi_I^s = \frac{1}{\kappa} \frac{1}{4\pi r(Q, \mathbf{s}_I)}$$

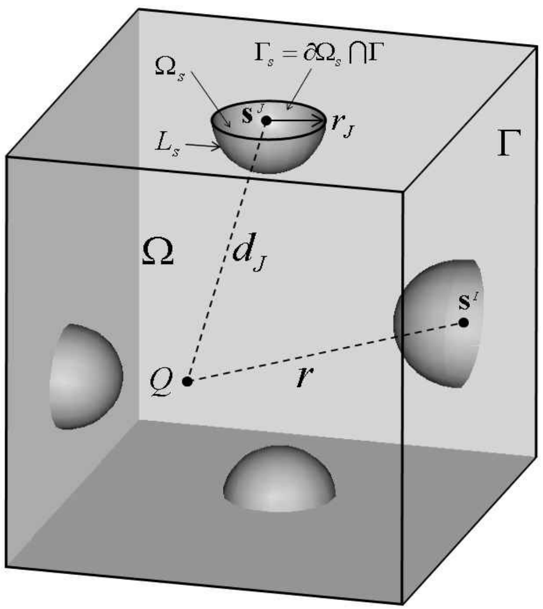
- Boundary variables

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

HBNM for single domain (3)

- **Local weak form**

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



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

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

HBNM for single domain (4)

➢ **System of equations – final form**

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

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

where

$$U_{IJ} = \int_{\Gamma_s^J} \frac{\partial \phi_I^s}{\partial n} v_J(Q)\, d\Gamma$$

$$V_{IJ} = \int_{\Gamma_s^J} \phi_I^s v_J(Q)\, d\Gamma$$

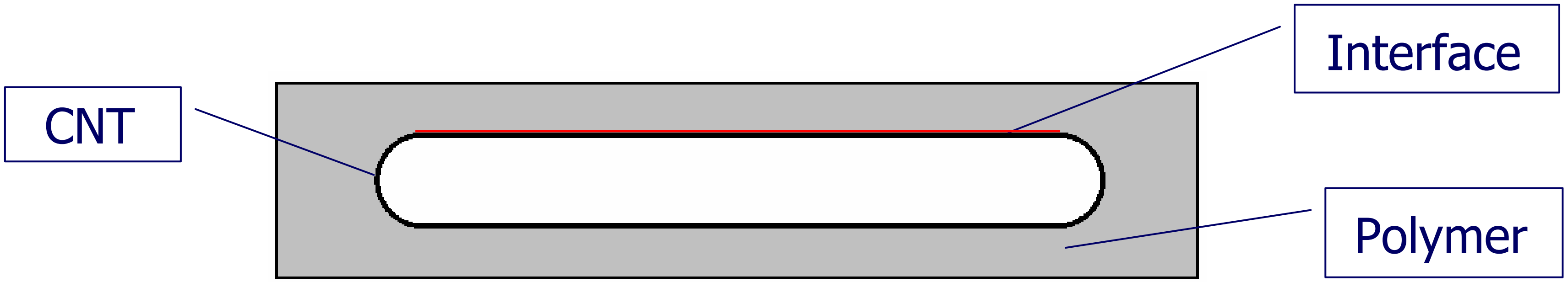
$$H_{IJ} = \int_{\Gamma_s^J} \Phi_I(\mathbf{s}) v_J(Q)\, d\Gamma$$

Multi-domain HBNM

- **CNT and Polymer**

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

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



Multi-domain HBNM (2)

- **Continuity and equilibrium at the interface**

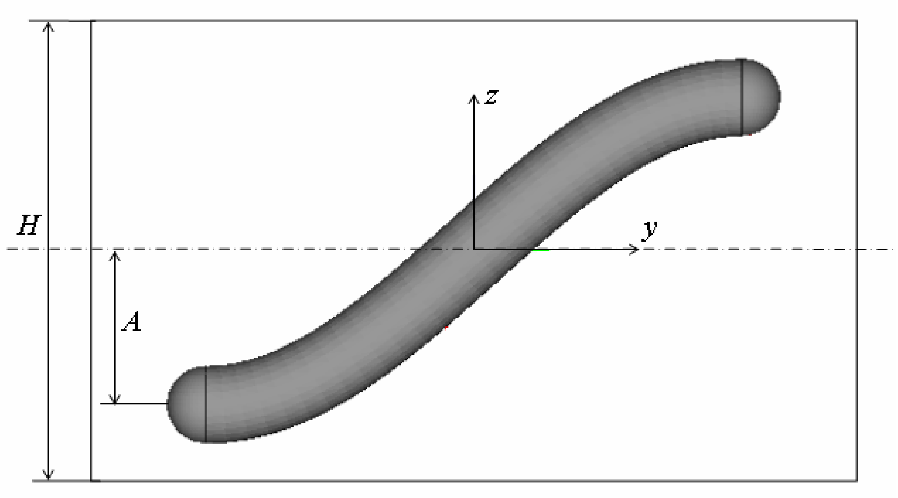
$$\left\{\phi_1^p\right\} = \left\{\phi_1^n\right\} \qquad \left\{q_1^p\right\} = -\left\{q_1^n\right\}$$

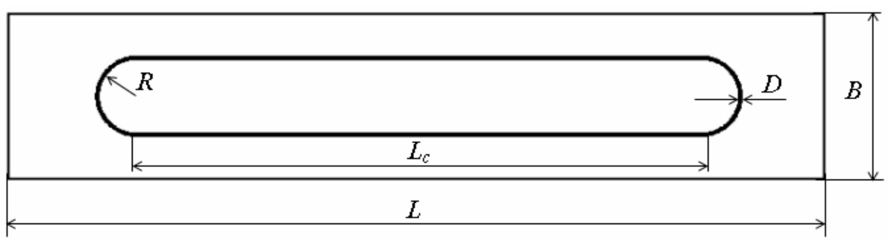
- **Assembled system of equations**

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

RVE with 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

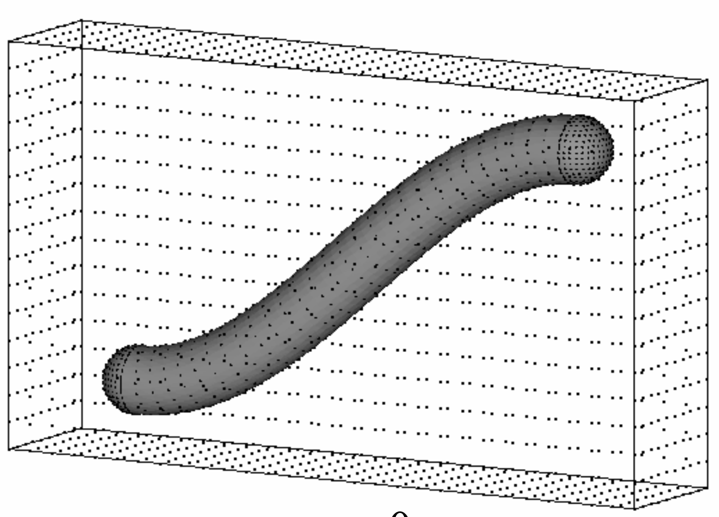
Conductivities

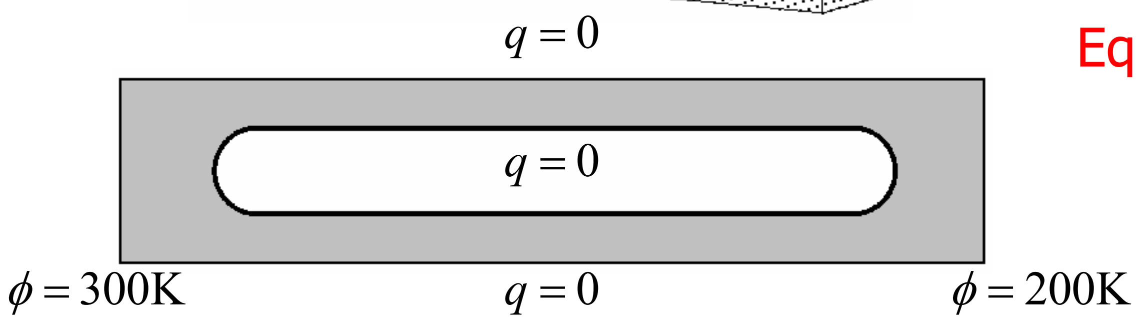
Nanotube: 6000 W/m·K

Polymer: 0.34 W/m·K

RVE with curved CNT (2)

- **Discretization and boundary conditions**





Polymer matrix: 2984 nodes

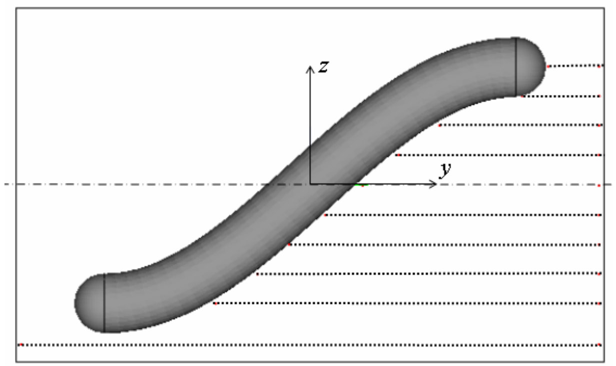
Carbon nanotube: 2208 nodes

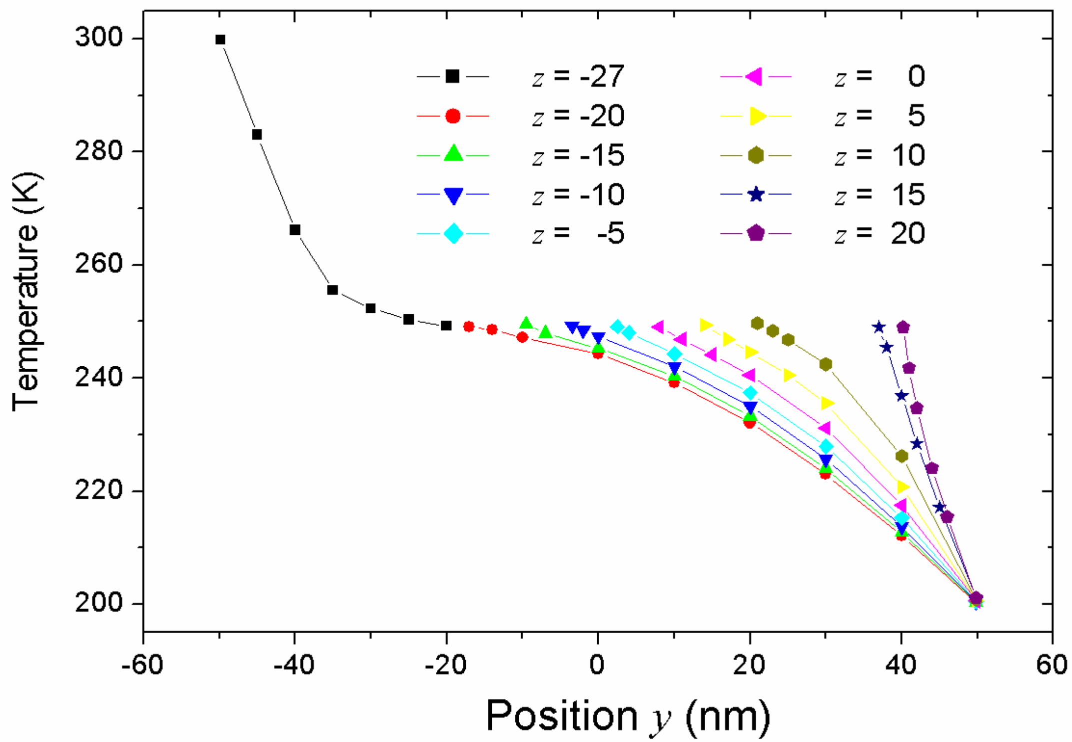
Equivalent heat conductivity

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

Results

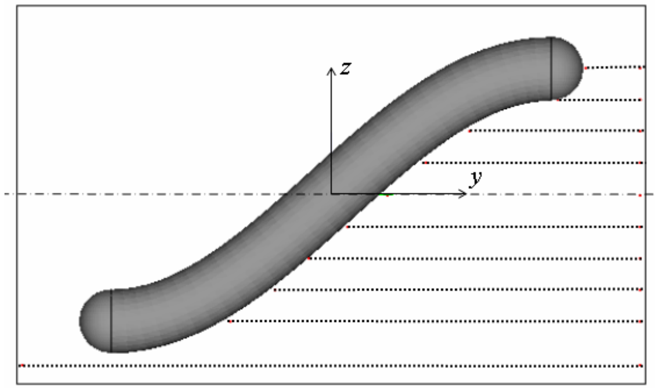
- **Temperature distribution**

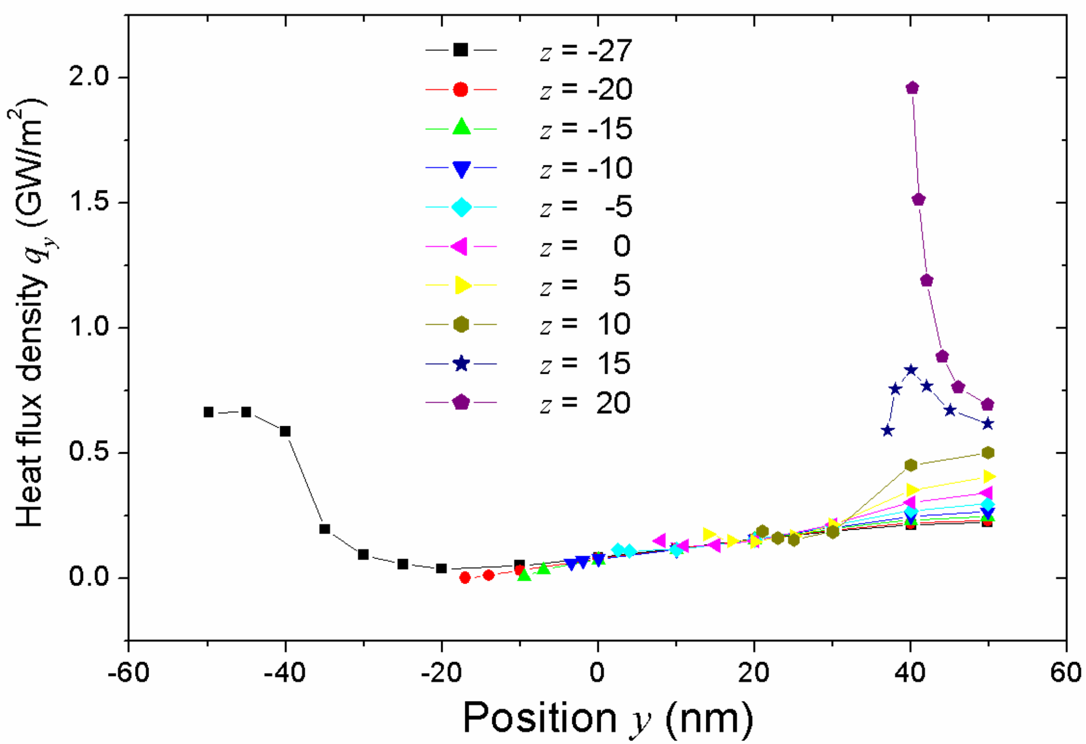




Results (2)

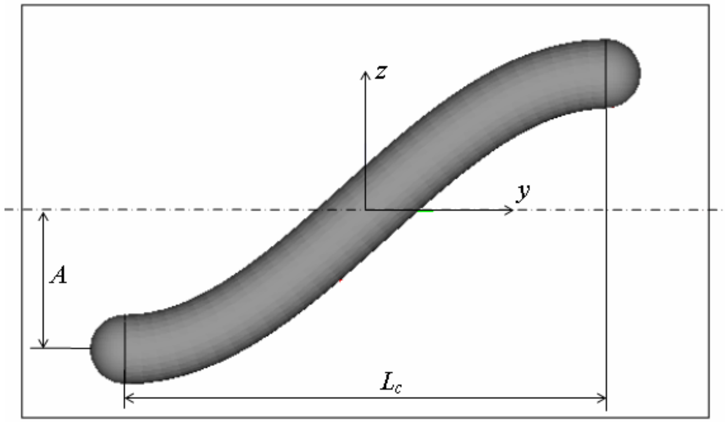
- **Flux distribution**



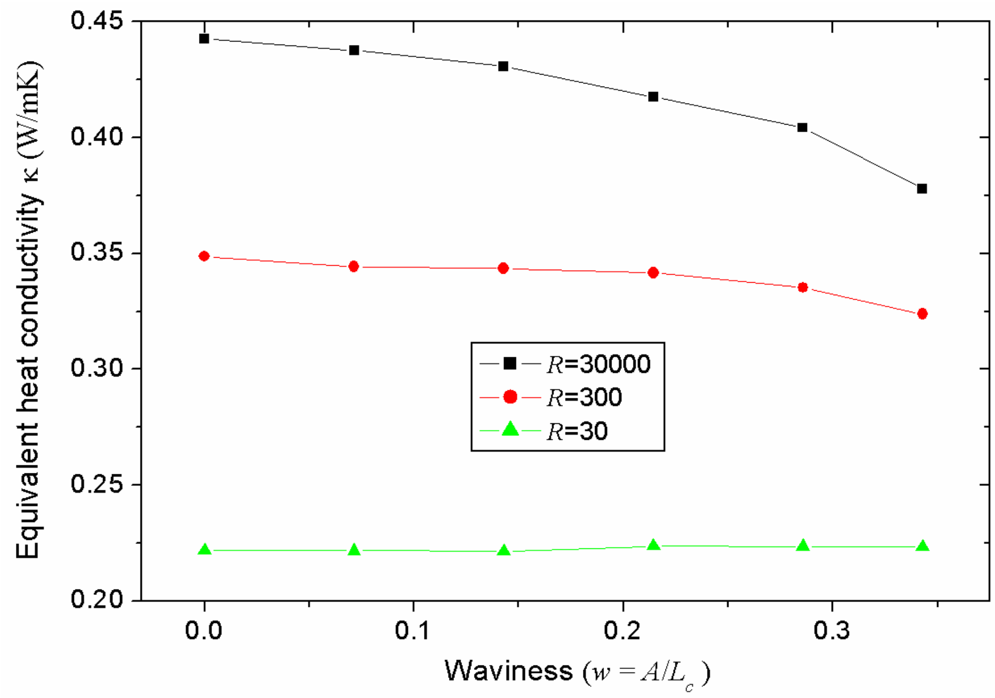


Results (3)

- **Equivalent heat conductivity**



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



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)
- The HBNM combined with FMM should be capable of solving an RVE containing many randomly distributed CNTs