Elastic and Piezoelectric Properties of Boron Nitride Nanotube Composites

Part II: Finite Element Model

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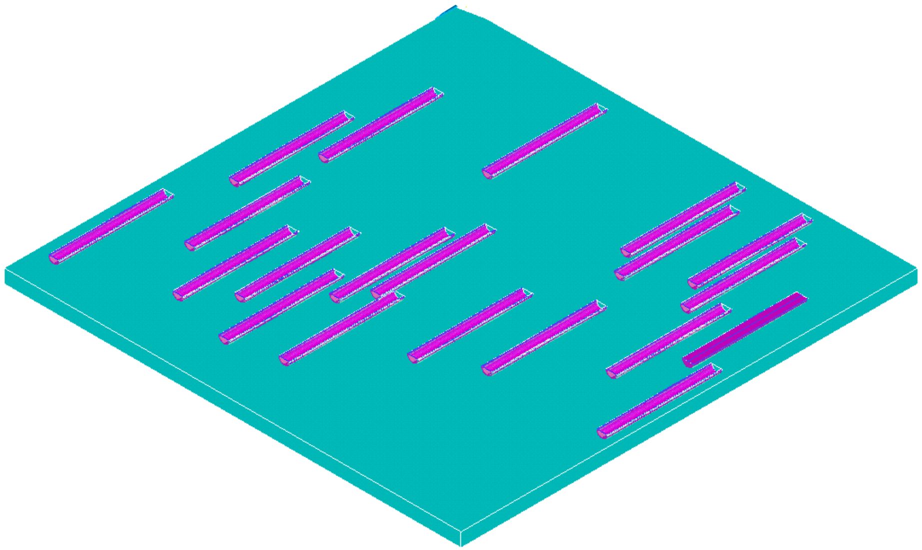
Background: Boron Nitride Nanotube (BNNT)

- Our interest is in piezoelectric properties.
- Nitrogen atoms are more electronegative than boron atoms.
- Polarisation is cancelled out due to chiral symmetry.
- Strain induces polarisation field.
- Polarisation creates electric charge across a nanotube.
- Inherently multiscale

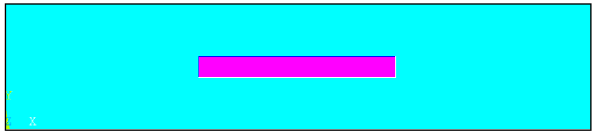
Research Aim

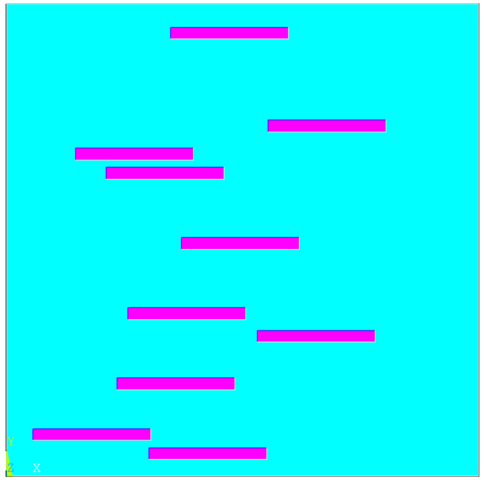
To investigate a suitable fidelity of a Representative Volume Element (RVE) Finite Element Model (FEM) of multiple Boron Nitride NanoTubes (BNNTs) in a matrix



2D FE Model

- Uniform distribution
- Random distribution





- Volume fraction

$$\frac{\text{Amount of stiff material (BNNT)}}{\text{Unit cell}}$$

- 2D area, 3D solid cylinder, 3D hollow tubes
- Reference – Analytical solution for finite length cylindrical inclusions at many orientations by Tandon and Weng (1976)

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Material Properties

Property	BNNT	Matrix Polymer
Young's modulus, E (GPa)	900	1.8
Poison's ratio	0.3	0.39
Axial piezoelectric constant, *e* (C/m^2)	0.2	-
Dielectric constant, *b* (pF/m)	159.3	79.6

Jafari et al. J Compos Mater 2013;47(16):1987–2003

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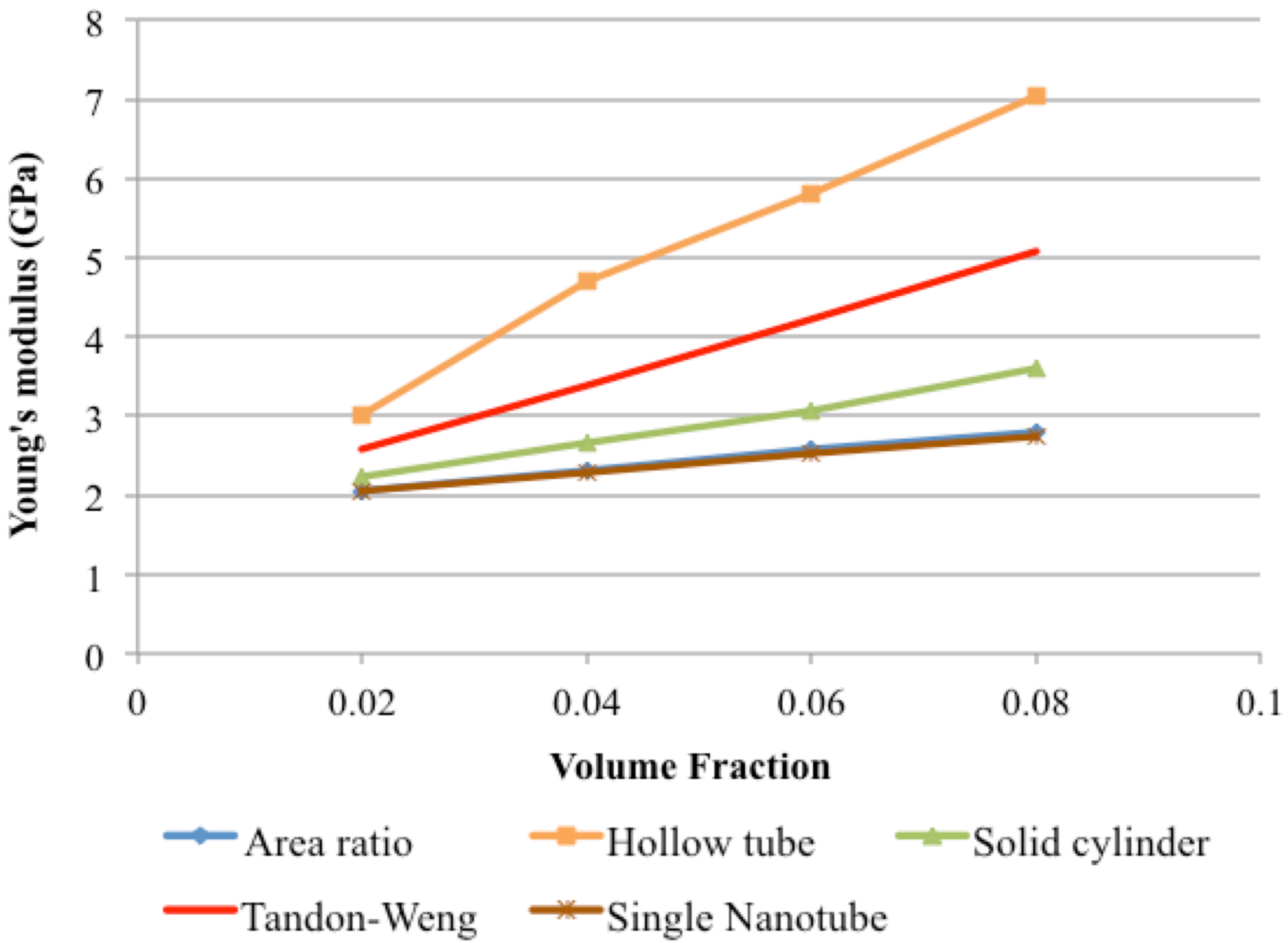
Elasticity Constant for 2D Models



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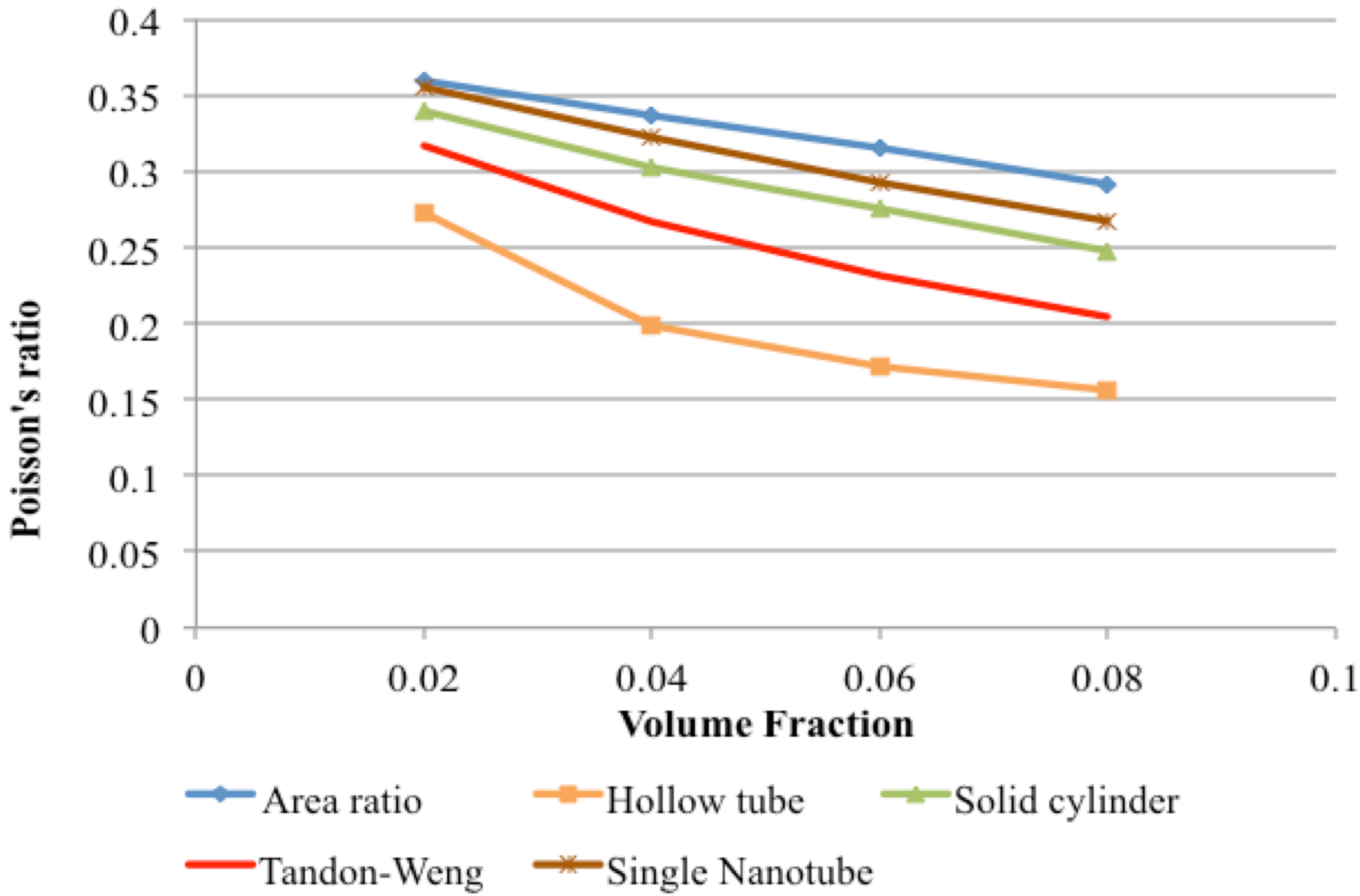
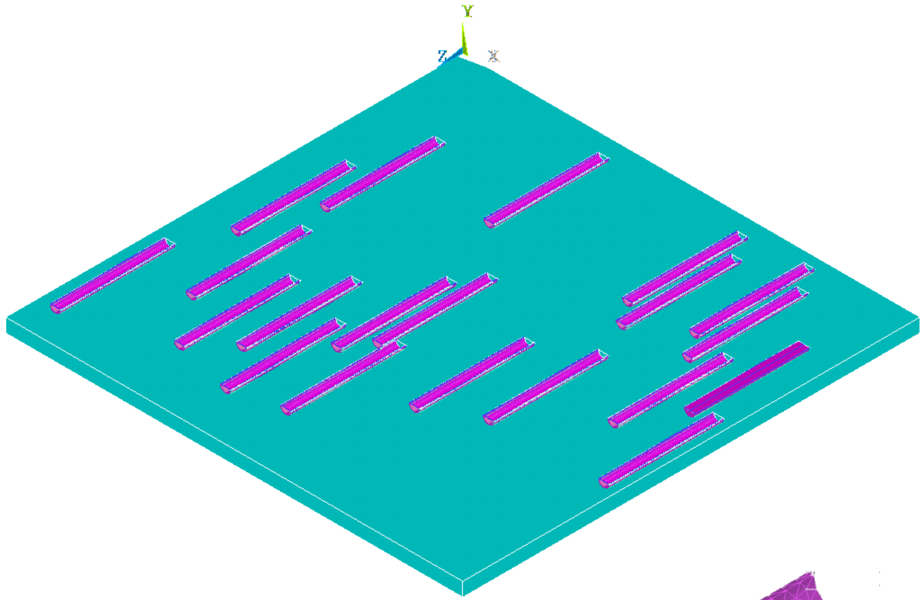
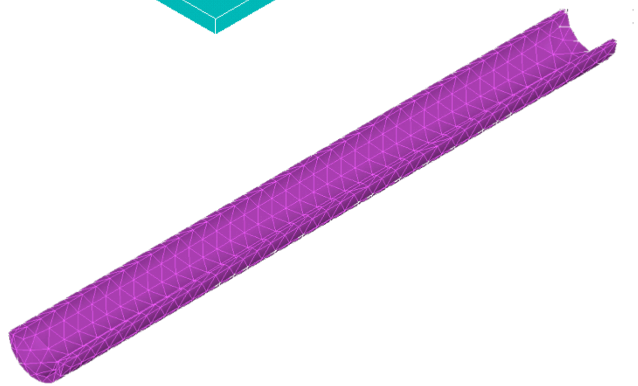
Elasticity Constant for 2D Models



3D FE Model

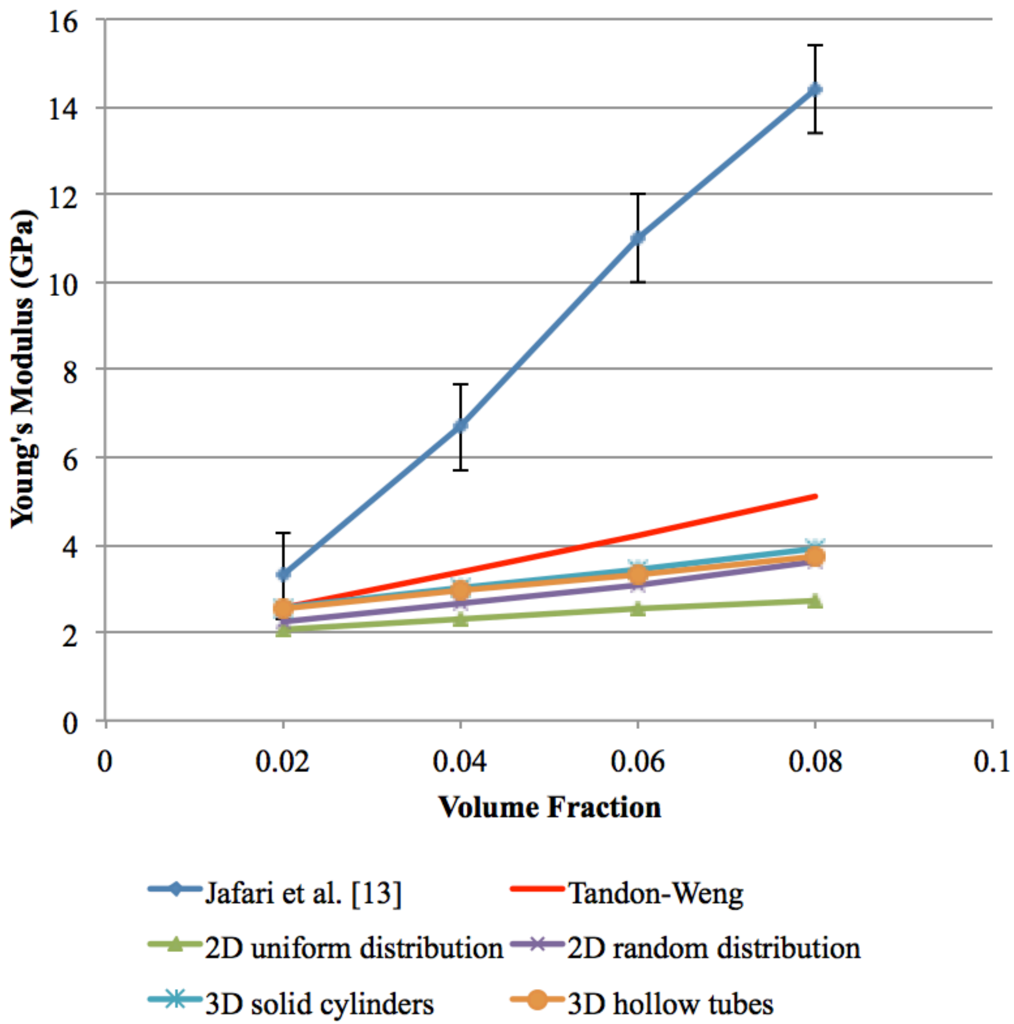
- Coupled field tetrahedral elements
- BNNTs modelled as:
    1) Solid cylinders
    2) Hollow tubes





$$\begin{Bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_{12} \\ D_1 \\ D_2 \end{Bmatrix} = \begin{bmatrix} C_{11}^* & C_{12}^* & 0 & -e_{11}^* & -e_{11}^* \\ C_{21}^* & C_{22}^* & 0 & -e_{11}^* & -e_{11}^* \\ 0 & 0 & C_{66}^* & -e_{11}^* & -e_{11}^* \\ & & & b_{11}^* & 0 \\ & & & 0 & b_{22}^* \end{bmatrix} \begin{Bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_{12} \\ E_1 \\ E_2 \end{Bmatrix}$$

Young's Modulus



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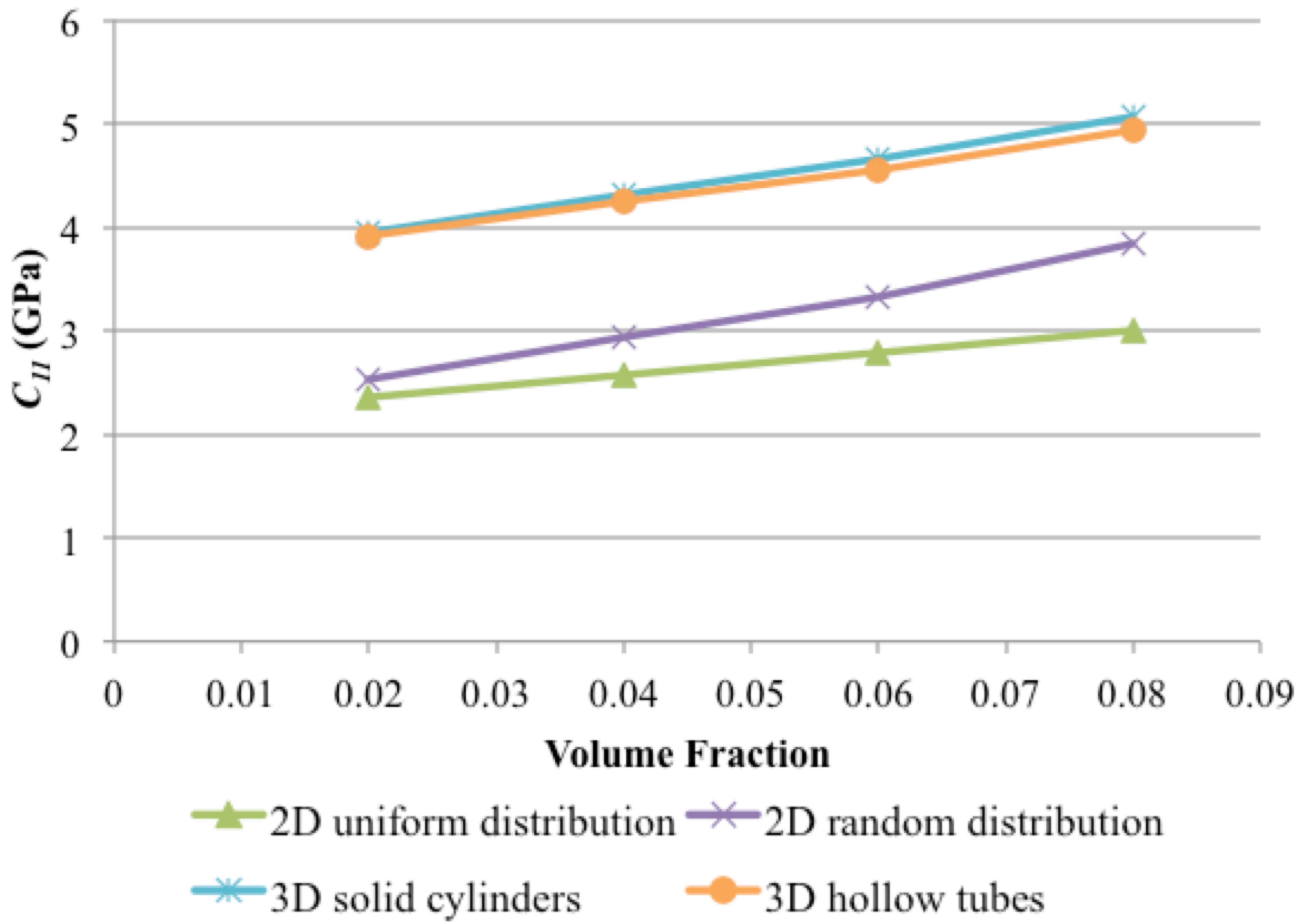
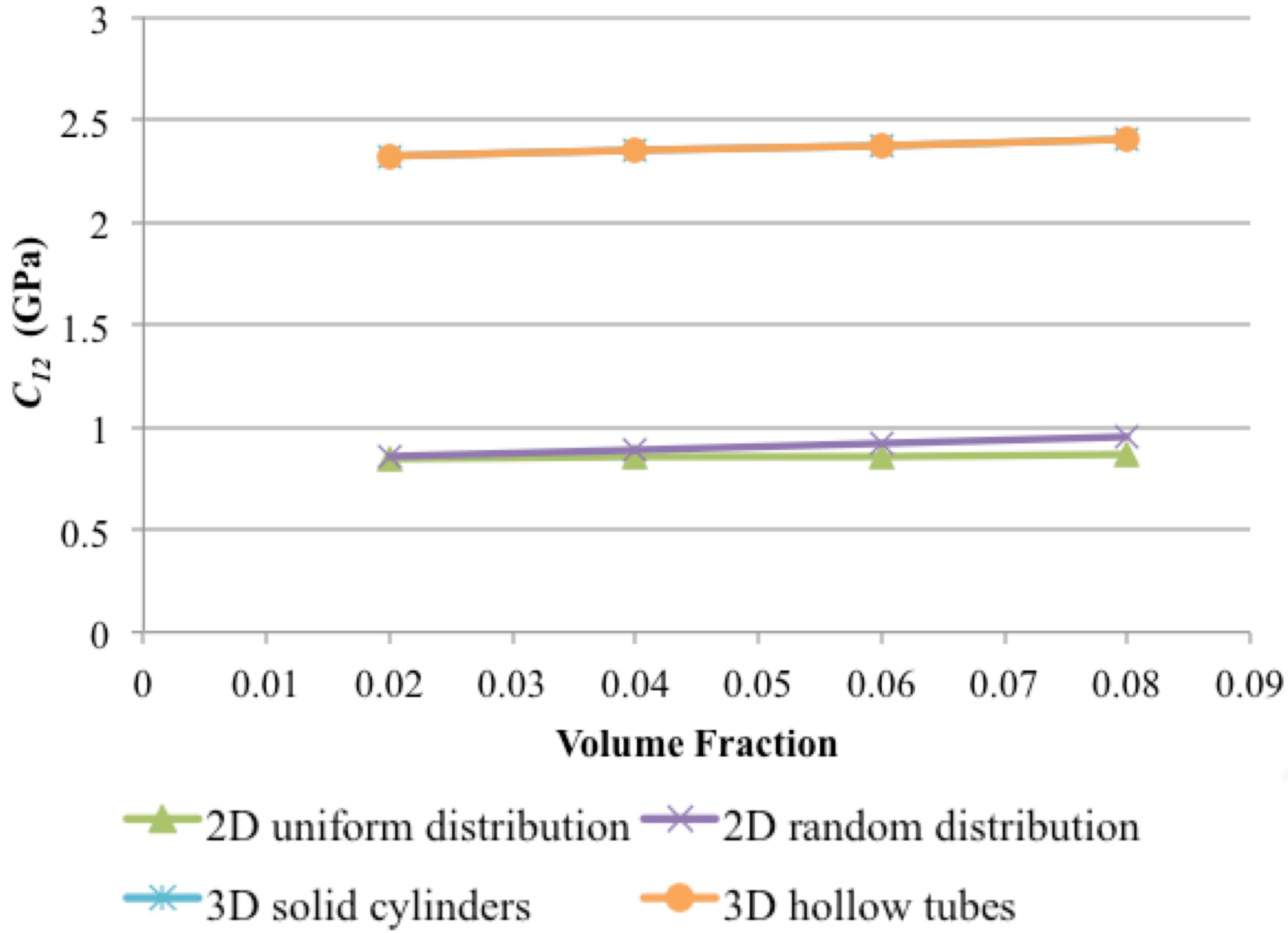
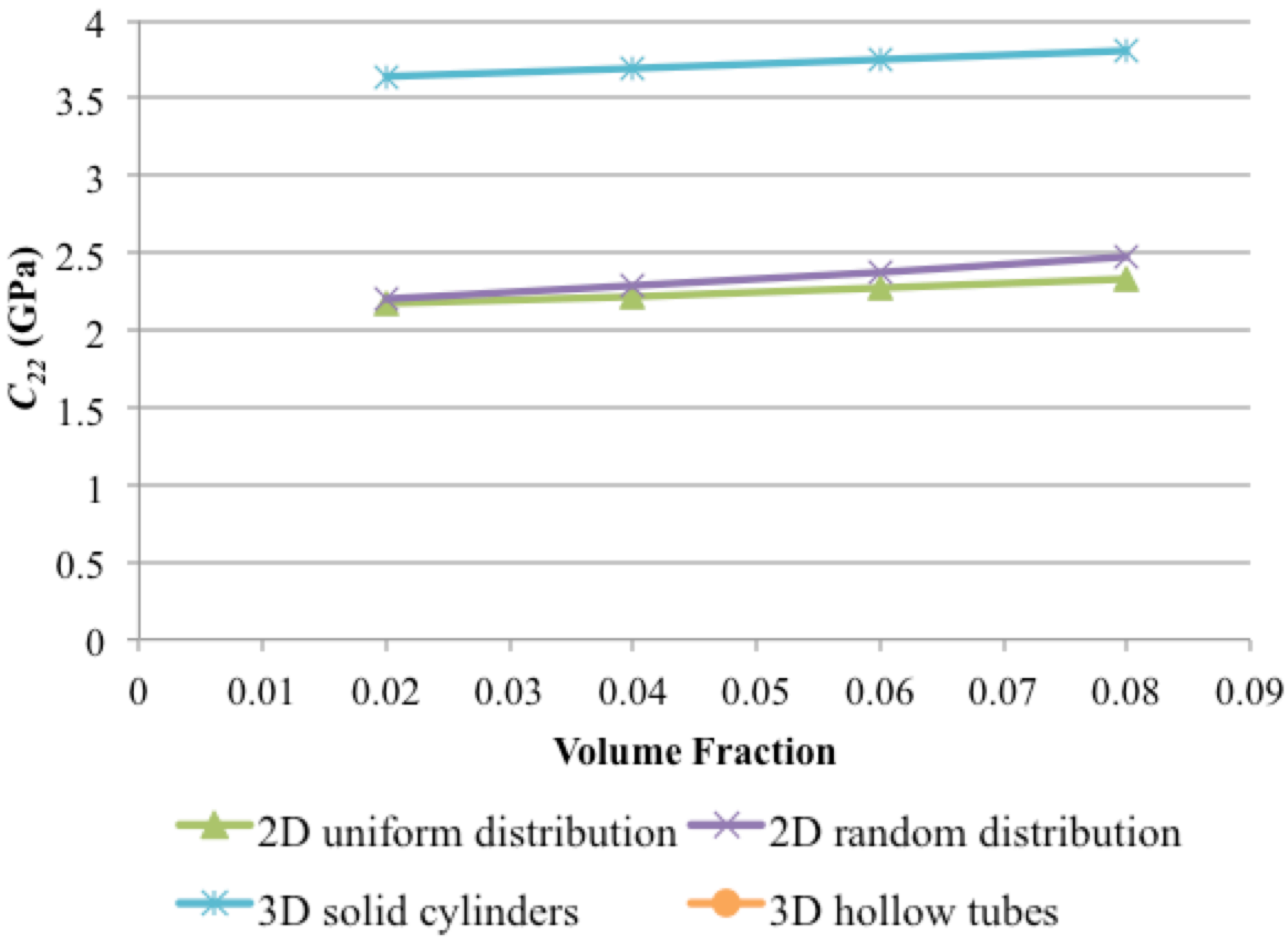
Elasticity Constant, C_{11}



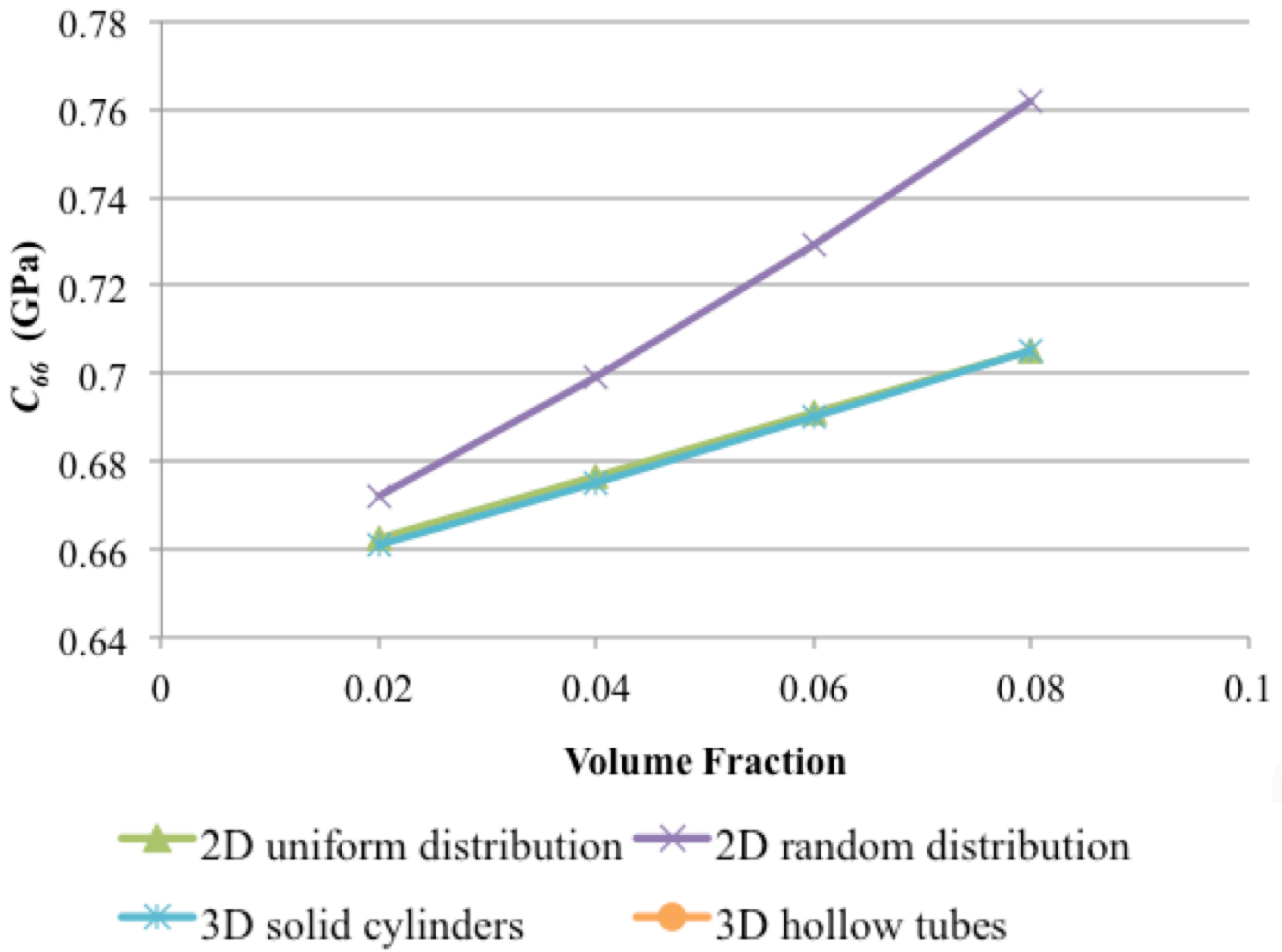
Elasticity Constant, C_{12}



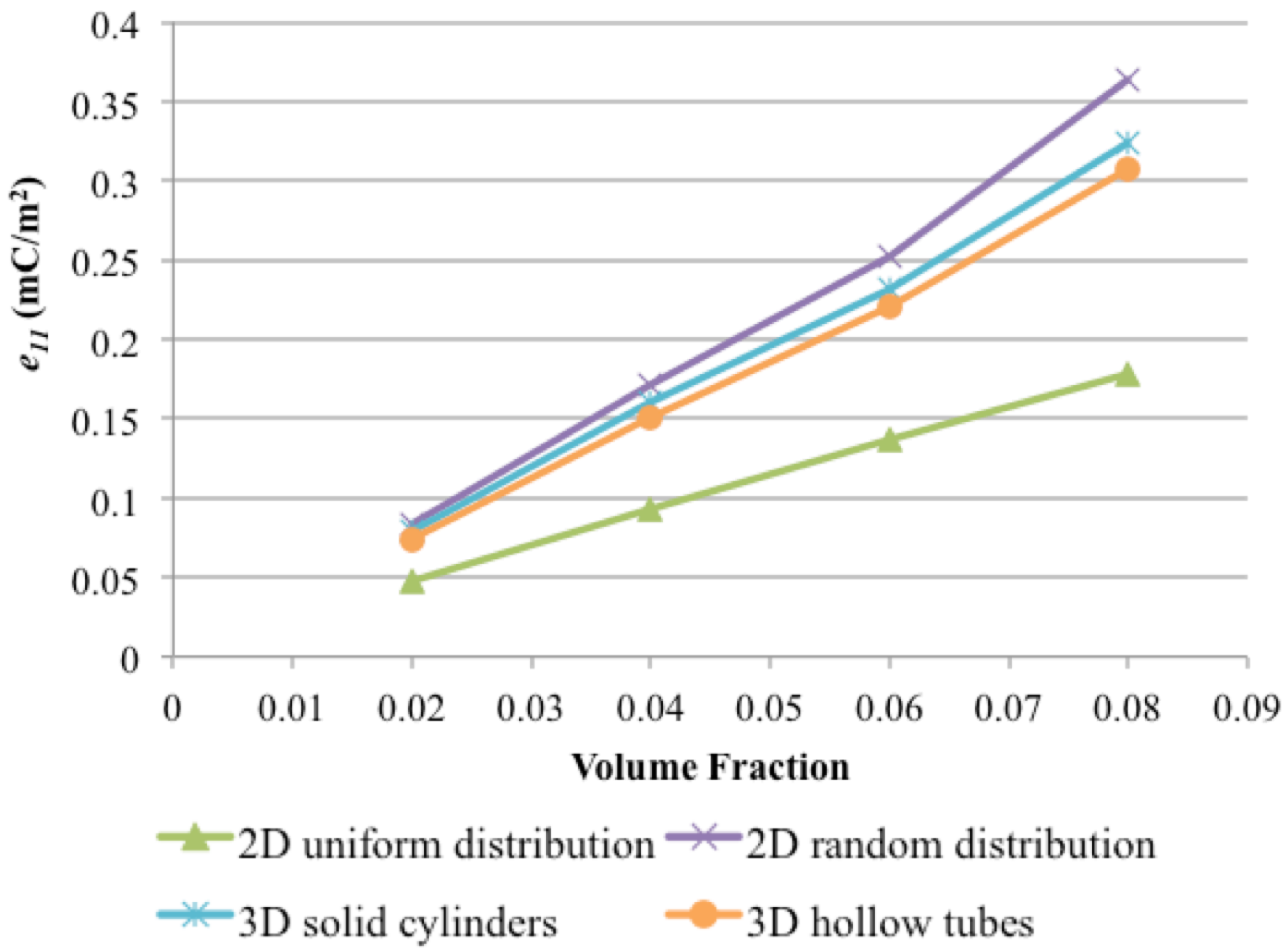
Elasticity Constant, C_{22}



Elasticity Constant, C_{66}



Piezoelectric Constant



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Conclusion

- 2D uniform distribution model can offer a first order understanding of the effective elastic and piezoelectric properties
- Volume fraction based on filled solids was most appropriate for 2D model
- Differences between 3D models with solid cylinders and with hollow tubes insignificant
- C_{11} and e_{11} most sensitive to the volume fraction