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
  
  \[
  \text{Amount of stiff material (BNNT)}
  \]
  
  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)
# Material Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>BNNT</th>
<th>Matrix Polymer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus, $E$ (GPa)</td>
<td>900</td>
<td>1.8</td>
</tr>
<tr>
<td>Poison’s ratio</td>
<td>0.3</td>
<td>0.39</td>
</tr>
<tr>
<td>Axial piezoelectric constant, $e$ (C/m$^2$)</td>
<td>0.2</td>
<td>-</td>
</tr>
<tr>
<td>Dielectric constant, $b$ (pF/m)</td>
<td>159.3</td>
<td>79.6</td>
</tr>
</tbody>
</table>

Elasticity Constant for 2D Models

Graph showing the Young's modulus (GPa) as a function of volume fraction for different models:
- Area ratio
- Hollow tube
- Solid cylinder
- Tandon-Weng
- Single Nanotube
Elasticity Constant for 2D Models

![Graph showing the relationship between Poisson's ratio and volume fraction for different models. The graph includes lines for Area ratio, Hollow tube, Solid cylinder, Tandon-Weng, and Single Nanotube.]
3D FE Model

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

\[
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_{12} \\
D_1 \\
D_2
\end{bmatrix} =
\begin{bmatrix}
C_{11}^* & C_{12}^* & 0 & -e_{11}^* & -e_{11}^* \\
C_{21}^* & C_{22}^* & 0 & -e_{11}^* & -e_{11}^* \\
0 & 0 & C_{66}^* & -e_{11}^* & -e_{11}^* \\
0 & 0 & b_{11}^* & 0 & 0 \\
0 & 0 & 0 & b_{22}^* & 0 \\
\end{bmatrix}
\begin{bmatrix}
\epsilon_1 \\
\epsilon_2 \\
\epsilon_{12} \\
E_1 \\
E_2
\end{bmatrix}
\]
Young’s Modulus
Elasticity Constant, $C_{11}$
Elasticity Constant, $C_{12}$
Elasticity Constant, \( C_{22} \)
Elasticity Constant, $C_{66}$
Piezoelectric Constant
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