MODELING OF ELECTRICAL CONDUCTIVITY IN CARBON NANOTUBE-BASED COMPOSITES

Chunyu Li (PD), Tsu-Wei Chou

University of Delaware . Center for Composite Materials . Department of Mechanical Engineering

CARBON NANOTUBE-BASED CONDUCTIVE COMPOSITES

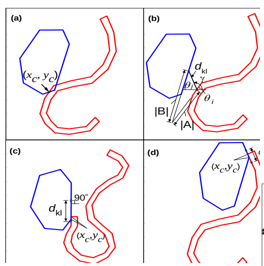
- **Carbon nanotubes have high electrical conductivity. They are expected to be ideal candidates for conductive composites because their high aspect ratio.**
- **Most of measured electric conductivities ranges from 10-5 to 10-2 S/m near percolation thresholds.**
- **But the electrical conductivity tailored to the range of 0.01~3180 S/m by varying the nanotube content from 0.11 to 15 wt% has also been reported.**

? The question is why the electrical conductivity of carbon nanotube composites varies in so large range.

Our Monte Carlo simulations try to reveal the effects of two main factors:

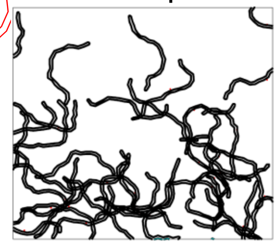
Nanotube wavines - Contact resistance

PERCOLATION OF ARBITRARILY SHAPED MULTIPLE-FILLERS



Fillers are approximated by polygons.

It is a versatile method for identifying percolation threshold in 2D nanocomposites



Nanotube network

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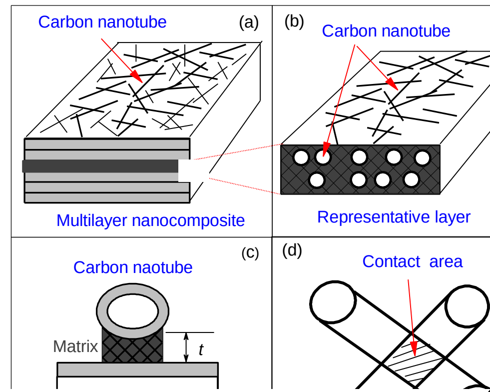
CONTACT RESISTANCE MODEL



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CONTACT RESISTANCE

$$R_C = R_{directcontact} + R_{tunnel}$$

The tunneling resistance depends on the thickness and material of the insulating layer.

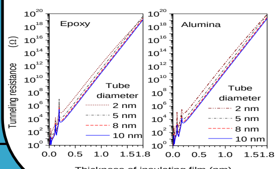
$$R_{tunnel} = \rho_{tunnel} / A_C$$

$$\rho_{tunnel} = U / J \qquad U = e / C = et / A_C K \varepsilon_0 \qquad A_C = d^2$$

$$J = 6.2 \times 10^{10} (\Delta t)^{-2} [\varphi \exp(-1.025 \Delta t \varphi^{\frac{1}{2}}) - (\varphi + U) \exp(-1.025 \Delta t (\varphi + U)^{\frac{1}{2}})]$$

$$\varphi = \varphi_0 - (U / 2t)(t_1 + t_2) - [5.75 / K \Delta t] \ln[t_2 (t - t_1) / t_1 (t - t_2)]$$

$$t_1 = 6 / K \varphi_0 \qquad t_2 = t(1 - 46 / (3\varphi_0 K t + 20 - 2UKt)] + 6 / K \varphi_0$$



The maximum tunneling gap in CNT-based composites is ~1.8 nm.

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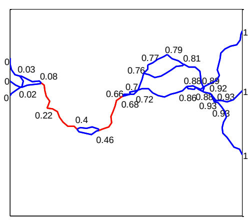
BACKBONE OF PERCOLATING NETWORK



Spanning cluster

Nodal voltage

Current in CNTs

Backbone

Effective conductance:

$$R_{eff} = (V_{right} - V_{left}) / I_{total} \qquad C_{eff} = 1 / R_{eff}$$

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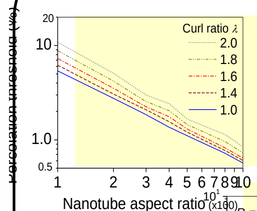
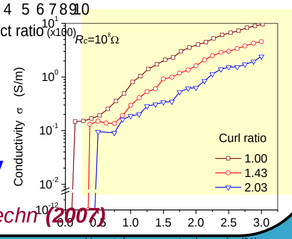
COMPOSITE CONDUCTIVITY



Percolation threshold deceases with large aspect ratio and straight nanotube.

Nanotube waviness reduces composite conductivity



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ACHIEVEMENTS

- Proposed a versatile method for identifying spanning clusters of arbitrary-shaped fillers;
- Developed an efficient backbone identification method (Direct Electrifying) ;
- Established a contact resistance model;
- The effect of nanotube waviness on electrical conductivity of nanotube-based composites was investigated.

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