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MULTISCALE MODELING OF MULTIFUNCTIONAL NANOCOMPOSITES: OPPORTUNITIES AND CHALLENGES

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In this keynote lecture, I shall present two multiscale modeling techniques that have successfully been developed in my laboratory to design multifunctional polymeric nanocomposites [1-4]. Mechanical, interfacial, electrical, and piezoresistive properties of carbon nanotube (CNT)-reinforced polymer composites were investigated using molecular dynamics (MD), micromechanics, and coupled electromechanical modeling techniques. Additionally, scanning electron microscopy and atomic force microscopy were used to determine the morphology and dispersion state of typical CNT-epoxy composites [2, 3]. Based on these measurements, realistic nanocomposite structures were modeled using representative volume elements (RVEs) reinforced by CNTs with different aspect ratios, curvatures, orientations, alignment angles, and bundle size. The obtained atomistic mechanical properties of the composite constituents were then scaled up using Mori-Tanaka micromechanical scheme. The outcome of the simulations revealed the following:

(i) the elastic modulus of a nanocomposite reinforced by well-dispersed straight CNTs increases almost linearly with the increase of their volume fraction,

(ii) the combined effect of CNT waviness and agglomeration results in a significant reduction in the bulk properties of the nanocomposite, and

(iii) the nanocomposites gauge factor as a sensor exceeds that of typical strain gauges and, as expected, is sensitive to the CNT concentration.

References

[1] A. R. Alian, S. A. Meguid, SI Kundalwal. Unraveling the influence of grain boundaries on the mechanical properties of polycrystalline carbon nanotubes, *Carbon*, 125:180-188, 2017

[2] MAN Dewapriya, SA Meguid. Tailoring fracture strength of Graphene. *Computational Materials Science*, 141: 114-121, 2018.

[3] S. A. Meguid. (Editor). Advances in Nanocomposites. *Springer Nature*, Amsterdam, 2016.

[4] S. A. Meguid and G. J. Weng (Editors). Micromechanics and Nanomechanics of Composite Solids. *Springer Nature*, Amesterdam, 2017.