MAR11-2010-002292

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Multiscale (atomistic to mesoscopic) modeling of carbon nanotube materials[1]

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A principal challenge in the development of computational models for investigation of collective dynamic phenomena in multi- component molecular systems or nanocomposites is presented by the gap between the atomistic description of the elementary structural units and the effective material behavior and properties. We approach this challenge through the development of computational models for dynamic simulations at intermediate (mesoscopic) length and time scales. An example of a mesoscopic model that is being currently designed in our group for carbon nanotube (CNT)-based materials and nanocomposites will be discussed in the presentation. The mesoscopic dynamic model for CNT materials is based on a coarse-grained representation of individual CNTs as chains of stretchable cylindrical segments [1] and a computationally-efficient "tubular potential" method describing the van der Waals interactions among the CNT segments [2]. Mesoscopic descriptions of CNT buckling and fracture are developed based on the results of atomistic simulations and incorporated into the model. Mesoscopic simulations performed for a system composed of randomly distributed and oriented CNTs predict a spontaneous self-assembly of CNTs into a continuous network of bundles with partial hexagonal ordering of CNTs within the bundles [2]. The structures produced in the simulations are similar to the structures of CNT films and mats observed in experiments. The first results illustrating the applications of the model for investigation of the response of CNT materials to dynamic mechanical loading, analysis of the structural dependence of the thermal transport properties [3] and gas permeability in CNT films will be briefly discussed in the presentation. Challenges and possible future directions in the development of a realistic mesoscopic description of nanocomposite materials will be outlined.

[1] L.V. Zhigilei, C. Wei, D. Srivastava, Phys. Rev. B 71, 165417, 2005.
[2] A.N. Volkov, L.V. Zhigilei, J. Phys. Chem. C 114, 5513, 2010; ACS Nano 4, 6187, 2010.
[3] A.N. Volkov, L.V. Zhigilei, Phys. Rev. Lett. 104, 215902, 2010.

[1]This work is supported by AFOSR (Grant No. FA9550-10-1-0545) and NSF (Grant No. CBET-1033919).