Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Mesoscopic model for CNT-based materials[1] ALEXEY VOLKOV, KIRIL SIMOV, LEONID ZHIGILEI, University of Virginia — A mesoscopic computational model is developed for simulation of the collective mechanical and thermal behavior of carbon nanotubes (CNTs) in CNT-based materials. The model is based on a coarse-grained representation of CNTs as "breathing flexible cylinders" consisting of a variable number of segments. A novel effective "tubular" potential is developed for the description of van der Waals inter-tube interactions. It accounts for the relative local orientation of the interacting CNT segments. Frictional forces and energy dissipation, as well as heat conduction along and between CNTs, are incorporated into the mesoscopic model and parameterized with the help of results from atomistic simulations. The developed model is used in calculations of the mechanical and thermal properties of CNT meshes and mats. The systems under consideration contain thousands of CNTs, allowing for investigation of the effective properties of CNT-based materials. The computational results are related to available experimental data.

[1]Support of this work is provided by NSF (NIRT-0403876) and NASA (NNX07AC41A)

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Date submitted: 21 Nov 2007 Electronic form version 1.4