

Abstract Submitted
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A coarse-grained model for simulations of graphite and carbon nanotubes ALPER BULDUM, Department of Physics, The University of Akron, Akron, OH 44325, TOSHIYUKI OHASHI, Honda Research Institute USA, Inc., Columbus, OH, 43212, LIMING DAI, Department of Chemical and Materials Engineering, University of Dayton — As multi-walled nanotubes in many experimental systems are quite large in diameter and in length and they consist billions of atoms, a new multi-scale modeling approach is necessary. This modeling approach can serve as a bridge between atomistic modeling and continuum modeling of multi-walled nanotubes. For graphite nanobeams and carbon nanotubes we present a new model which is based on the hexagonal symmetry of the graphite structure. This model is based on “N cell to one Cell” mapping of the graphite structure. N cells in the original atomic structure are equivalent to one cell in the hexagonal mesh model. The number N can be very large thus it is possible to model large multi-walled nanotubes and graphite nanobeams.

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