

Computational design of carbon nanotube network materials and polymer matrix nanocomposites

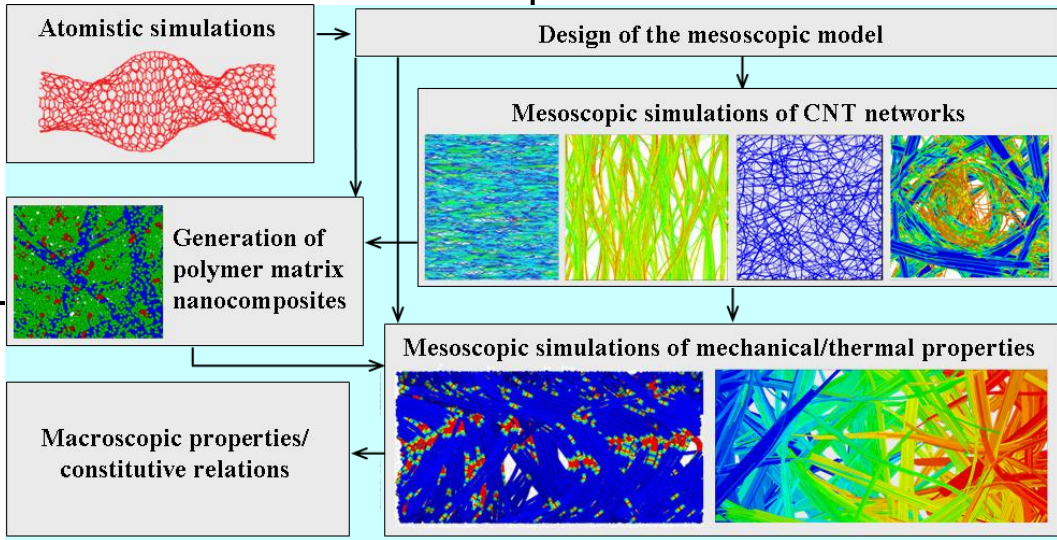
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Research Objectives

Develop an advanced mesoscopic model for CNT materials and nanocomposites

Perform systematic analysis of the structural, mechanical and transport properties of the CNT materials



Approach

mesoscopic model for CNT networks and nanocomposites

- Shape-based mesoscopic model for nanotubes/nanoribbons
- Smooth Particle Hydrodynamics and coarse-grained molecular representations of polymer matrix
- Cross-links, chemical functionalization, defects
- Parameterization based on atomistic simulations

Potential Impact

Development of a robust mesoscopic model will facilitate the development of multifunctional low-density materials with unique combination of mechanical and transport properties tailored for aerospace applications.