Multiscale modeling and analysis of nanofibers and nonwoven materials

OVERVIEW: Electrospinning has emerged in recent years as a promising method for producing nanofibers and macroscale collections of nanofibers (nonwovens). [1] But it’s hard to measure single fiber properties due to small fiber sizes, while nonwoven properties are complicated by numerous super-fibrillar mesh-related properties, such as fill fraction, fiber-fiber contact interactions, fiber stiffness and orientation. The overall goal of this project is to develop the necessary modeling tools to characterize and quantify the size dependence of polymeric materials in one-dimensionally (1-D) confined geometries, in particular nanofibers, and to relate the nanofiber properties to the properties of nonwoven fabrics.

OBJECTIVES:
- Analysis of single nanofiber behavior by Molecular Dynamics (MD) (nanometer level) and multiscale modeling (submicron level)
- Implementation of a simulation technique for nonwoven materials based on molecular modeling algorithms and evaluation of the behavior of nonwoven materials (continuum level)
- Establishing the connection between fiber and nonwoven fabric length scales and calculation of the mechanical and transport properties of nonwoven fiber networks using the data from single nanofiber MD simulation

APPROACH:
We are using molecular dynamics (MD) for the simulation of nanofibers. Current computer speeds are practically limited to studies of O(5000 atoms) and O(10 ns) for molecular dynamics on a single CPU. Our solutions to this problem include parallel MD methods [2] and coarse-graining [3]. In this way, we plan to simulate realistic size fibers. For modeling of nonwoven mats, algorithms to construct models of chain-like molecules that take into account both intramolecular and intermolecular interactions will be used, by analogy, to construct models of thread-like fibers with intra-fibrillar (e.g. bending stiffness) and inter-fibrillar (e.g., surface charge repulsion) interactions.

NANOFIBER RESULTS:
(A) Radial density profiles from various systems show that the fibers show bulk-like behavior at the center and density decreases sigmoidally towards the surface.
(B) Energy density profiles are shown in Figure B. (C) Interfacial excess free energy was calculated according to Gibbs Dividing Surface Method. It was found that interfacial excess free energy is dependent on fiber size. For fibers that are mostly surface (Rfiber < 2 x interfacial thickness), energy increases to very high values compared to larger fibers.

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E_{\text{int}} = \int_{-\infty}^{\infty} (E_{\text{total}} - E_{\text{GDS}}) \, 2\pi r \, dr = 2\pi L \int_{0}^{R_{\text{bulk}}} E(r) \, r \, dr - \pi \sigma_{\text{bulk}} \pi R_{\text{div}} L
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References: