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Molecular Simulation of Size-Dependent Properties of Polymeric Nanofibers SEZEN CURGUL, GREG RUTLEDGE, KRYSTYN VANVLIET, MIT — Materials with nanometer dimensions have been shown experimentally to exhibit size dependent properties. Polymer nanofibers, in particular, are of interest because of their several value added applications such as medical, filtration, barrier, wipes, personal care, composite, garments, insulation, and energy storage. We report here the results of molecular dynamics (MD) simulations of polymer nanofibers using LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator). To date, we have simulated fibers comprised of chains that mimic the prototypical polymer polyethylene, with chain lengths ranging between C50 and C300. These nanofibers have diameters in the range 1.86-16.2 nm. The fibers have been analyzed for signature of size dependent behavior in their structural and dynamical properties. In these fibers, mass and energy density profiles are similar and they have constant bulk-like values at the center of the fiber, for sufficiently large diameter fibers. The surface layer thickness shows little dependence on the fiber size. The interfacial excess energy increases with decreasing fiber size for fibers below 5 nm in diameter. The chains at the surface show preferred conformations and orientations that are significantly different than chains at the center of the nanofiber.

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