Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Structure and Dynamics of Polymer / Single Wall Carbon Nanotube Nanocomposites NIGEL CLARKE, ARGYRIOS KARATRANTOS, University of Sheffield, KAREN WINEY, RUSSELL COMPOSTO, University of Pennsylvania — We simulate the static[1] and dynamic[2] properties of monodisperse polymers in the presence of a SWCNT using molecular dynamics. The SWCNT has a large aspect ratio and radius smaller than the polymer radius of gyration. We find that although the local chain structure is significantly affected, the overall configuration, as characterized by the radius of gyration, is not perturbed by either the interaction strength between the polymer and the SWCNT or by variations in the SWCNT radius. In contrast, for the dynamics of entangled polymers, we find a significant heterogeneity, with the center of mass polymer diffusion being affected by the strength of the enthalpic interaction between monomers and the SWCNT, as well as the SWCNT radii. In addition, we find that the polymer chain diffusivity perpendicular to the SWCNT is smaller than that parallel to the SWCNT in the case of entangled polymers.

[1]Karatrantos A., Composto R.J., Winey K.I., Clarke N., Macromolecules, accepted.
[2]Karatrantos A., Composto R.J., Winey K.I., Clarke N., in preparation.

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Date submitted: 26 Nov 2011 Electronic form version 1.4