

Engineering Conferences International ECI Digital Archives

Composites at Lake Louise (CALL 2015)

Proceedings

Fall 11-9-2015

Polymer melts inside nanoscale cylindrical pores: Chain conformations, polymer diffusion and local dynamics

Karen Winey
University of Pennsylvania

Follow this and additional works at: http://dc.engconfintl.org/composites_all

 Part of the [Materials Science and Engineering Commons](#)

Recommended Citation

Karen Winey, "Polymer melts inside nanoscale cylindrical pores: Chain conformations, polymer diffusion and local dynamics" in "Composites at Lake Louise (CALL 2015)", Dr. Jim Smay, Oklahoma State University, USA Eds, ECI Symposium Series, (2016). http://dc.engconfintl.org/composites_all/6

This Conference Proceeding is brought to you for free and open access by the Proceedings at ECI Digital Archives. It has been accepted for inclusion in Composites at Lake Louise (CALL 2015) by an authorized administrator of ECI Digital Archives. For more information, please contact franco@bepress.com.

Polymer Melts inside Nanoscale Cylindrical Pores: Chain Conformations, Polymer Diffusion and Local Dynamics

Karen I. Winey
University of Pennsylvania

ABSTRACT

Polymers in composites and inside porous media are frequently confined to spaces that are comparable to or even smaller than their mean end-to-end distances in the unconfined bulk state. Understanding the impact of nanoscale confinement on both polymer structure and dynamics is critical for a variety of applications including hydraulic fracturing fluids, porous inorganic thin films in the electronics industry, and composites. To date, our work focuses on polymer melts under nanoscale cylindrical confinement. The polymer center-of-mass diffusion into cylindrical pores in anodized aluminum oxide membranes (diameters 18 – 80 nm) was measured using elastic recoil detection. This ion beam method that provides the concentration profile of deuterated polystyrene (400 kg/mol) penetrating into the AAO membranes prefilled with polystyrene (200 or 290 kg/mol). The polymer diffusion coefficient increases with decreasing pore diameter. This experimental finding is corroborated by coarse grain simulations with neutral interactions with the pore walls, although the increase is more pronounced in the simulations. The simulations previously found that chain conformations slightly elongated parallel to the cylinder axis and compressed perpendicular to the cylinder and the number of entanglements per chain decreases as the cylinder diameter decreases. It is primarily the reduction in polymer entanglements that allows polymers to diffuse faster when the pore diameter is smaller. We have also probed the local polymer dynamics using quasi-elastic neutron scattering.