Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Effects of Morphology on Dynamics of Block Copolymer Systems[1]

KUAN-HSUAN SHEN, LISA HALL, Ohio State Univ - Columbus — It is well known that block copolymers can microphase separate into ordered structures such as lamellae, hexagonally packed cylinders, or the bicontinuous double gyroid phase. Understanding the dynamics of the chains themselves and of added selective small molecule penetrants is relevant to the design of polymeric systems for transport applications. We expect that chain and penetrant dynamics are strongly dependent on morphology, while chain dynamics are also significantly impacted by individual polymer conformations within the morphology. For instance, in prior work on tapered polymers with a midblock of various concentration profiles, chains that fold back and forth across the lamellar interface were shown to have significantly decreased diffusion. Here we use coarse-grained molecular dynamics simulations to study how chain and penetrant dynamics depend on domain spacing, polymer conformations, and microphase morphology. We initialize systems of various fractions of A monomers in lamellar, cylinder, or gyroid microphases by growing polymers in a constrained random walk such that the two blocks are placed on opposite sides of the interface. We include, for comparison, systems with the same fraction of A that are initialized (and kinetically trapped) in different microphases, and show how this impacts polymer relaxation. How the dependence of penetrant diffusion on morphology relates to that of polymer chains will also be discussed.

[1]This material is based upon work supported by the National Science Foundation under Grant 1454343.

Kuan-Hsuan Shen
Ohio State Univ - Columbus

Date submitted: 10 Nov 2016 Electronic form version 1.4