MAR17-2016-020342

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Three dimensional characterization of polymer nanostructures through an integrated scattering and modeling approach

MANOLIS DOXASTAKIS, Univ of Tennessee, Knoxville

Modern scattering techniques such as resonant X-ray and grazing-incidence small-angle X-ray scattering offer an unprecedented ability to quantitatively characterize nanoscale polymer structures on a substrate or embedded within thin films. In the case of line gratings or polymer lamellae formed by directed-self assembly, if the long structures are arranged with a nanoscale periodicity perpendicular to the beam, then scattering is concentrated into a series of characteristic spots recorded on a two-dimensional detector. The intensity of these spots is modulated by the three-dimensional shape and arrangement of the lines. However, data analysis is often focused onto extracting a two-dimensional model for the sample cross-section, discarding any additional information that the measurements can provide. In this talk, we will discuss how to leverage methods to extract details on the three-dimensional structure of such soft materials using a concerted computational and experimental approach. We will demonstrate the necessity to implement an efficient modeling strategy that maximizes output from such state-of-the art experimental techniques. Furthermore, by coupling molecular simulations to scattering we provide estimates on the thermodynamic and kinetic factors driving structure formation that are otherwise inaccessible. This combined modeling and scattering method is critical to probe and control processes central in the development of the next generation materials in nanopatterning.