Supporting Information for ChemPhysChem Z18:

Hydrophilic/Hydrophobic Nanostripes in Lipopolymer Monolayers

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To locate the ordered tails in the lipopolymer monolayer, specular X-ray reflectivity experiments were performed using a home-built apparatus.[1–3] Specular reflection provides information on the electron-density variation (scattering length density variation) perpendicular to the surface to an Ångström resolution. Due to the loss of phase information in conventional X-ray reflectivity experiments, the data analysis is generally based on finding proper electron-density functions, whose reflectivity properties best match, retrospectively, the observed reflectivity data. To obtain the optimum interfacial electron-density variations, we used two different strategies.

a) The layer is subdivided into homogeneous slabs (“box model”).[4] Each box is parameterized by a length and an electron density. The transition between adjecent boxes is smoothed. Proper smearing parameters describe the interfacial roughness (the roughness has the same effect as the Debye–Waller factor; it damps the interference maxima at large values of Q_z). The parameters are determined by a least-squares method. Box models are convenient because they are easy to integrate and individual boxes may be identified with certain structural properties of the layers. For more complex electron-density profiles however, many boxes are necessary to suitably describe the experimental data. This may necessitate the determination of more adjustable parameters than one can unambiguously deduce from the reflectivity data and various sets of parameters may result in the same electron-density

profile, within experimental error.[3, 5, 6] To recognize coupled parameters, an interdependency analysis was performed.[7]

b) The electron-density profile is determined with a model-independant method.[8, 9] From the experimentally determined reflectivity curve, the corresponding profile correlation function is estimated via an indirect Fourier transformation. For this profile correlation function, the matching scattering length density profile is then derived by square-root deconvolution. Both the correlation function and the density profile are expressed in terms of a linear combination of a set of suitable basis functions. The number of basis functions and, thus, that of free parameters, can be optimized (minimized) by smoothness criterion for the correlation function and, in most cases, no a priori assumptions on the shape of the electron-density profile have to be made.

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