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Modeling neutron scattering in disperse, nonuniformly labeled commercial polyolefins BRIAN HABERSBERGER, KYLE HART, DAVID GILLESPIE, TIANZI HUANG, Dow Chemical Co — In spite of their chemically simple monomer elements, understanding of many structural, thermodynamic, and other aspects of polyolefins has remained elusive. Scattering studies on polyolefins are challenged by their nearly identical density in the melt, requiring the use of deuterium-labeling to provide contrast for small-angle neutron scattering (SANS). Until recently, labeling of commercial polyolefins has been prohibitively costly, leading SANS investigations on polyolefins to focus on non-disperse model systems. Commercial polyolefins often have broad molecular weight and composition distributions, and such dispersity plays an important role in their rheology, crystallization, and mechanical properties. Recent reports have described facile hydrogen-deuterium exchange reactions that preserve the chain architecture of polyolefins. However, such exchange is not uniformly distributed across the chain population. Here, we report a generalized application of the Random Phase Approximation prediction for SANS from homogeneous polymer blends to account for such dispersity. A Monte-Carlo method is used to calculate the deuterium distribution that corresponds to SANS measurements. These methods provide powerful tools for probing the structure of disperse polymer architectures.

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