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Predictive Morphology Models for Crystalline Polymers[1] JACOB HARVEY, ZHICHENG XIAO, YVONNE AKPALU, Department of Chemistry & Chemical Biology, Rensselaer Polytechnic Institute — Modeling of small-angle scattering data provides information on heterogeneities on sizes on the order of 10 Angstroms and larger. The typical size, shape and arrangement of the heterogeneity can be determined by applying models to the scattering intensity $I(q)$. When there is a distribution in the size of structures present and when a system is densely packed, it is likely that models that can be used for analysis may not provide a unique description of the structure. With the recent interest developing predictive models for molecular level control over the properties of polymers, it is desirable to determine all unique structural and morphological contributions to a scattering curve without assuming a model. However, by using a multi-scale approach (i.e. light and X-ray scattering spanning multiple size scales), it may be possible to build unique models for crystalline polymers. We will show that hybrids of statistical methods can be used to decouple scattering data into unique structural components. We will show how our approach can be used to discover analytical models and to develop a set of descriptors that can be used to predict scattering curves for several other polymers that share a similar structure or crystallization condition.

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