

Abstract Submitted
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Percolating bulk-heterostructures from neutron reflectometry and small angle scattering data¹ DANIEL OLDS, PHILLIP DUXBURY, Michigan State University — We present a novel algorithm for efficiently calculating the simulated small angle scattering data of any discretized morphological model of arbitrary scale and resolution, referred to as the distribution function method (DFM). Unlike standard SAS fitting methods, the DFM algorithm allows for the calculation of form factors and structure factors from complex nanoscale morphologies commonly encountered in many modern polymeric and nanoparticle based systems, which have no exact analytical corollary. The computational efficiency of the DFM algorithm suggests it's use in morphological model refinement. We will present a number of simple examples to demonstrate the accuracy and limits of the algorithm, followed by an example of incorporation of the DFM algorithm into reverse Monte Carlo structural refinement of bulk-heterojunction two-phase morphologies, such as those commonly found in organic photovoltaic devices. We will show that morphological features introduced via direct incorporation of experimental neutron reflectometry and SANS data to the models has a direct effect on the results of device simulations.

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