

Abstract Submitted  
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**Three-Dimensional Characterization of Block Copolymers using Molecular Simulation and Small-Angle X-ray Scattering**<sup>1</sup> ALEC BOWEN, University of Chicago, MANOLIS DOXASTAKIS, University of Tennessee, GURDAMAN KHAIRA, Mentor Graphics Corporation, PAUL NEALEY, JUAN DE PABLO, University of Chicago — Block copolymers have gained considerable interest for their ability to spontaneously form vast arrays of nanoscale structures, which is of particular use in semiconductor manufacturing and membrane fuel cell applications. However, these materials typically rely on precise substrate patterns and composition control to form ideal structures. A fully three-dimensional characterization technique is necessary for understanding the relationship between thermodynamic process conditions and resultant nano-structures, and consequently fine-tuning them into their desired form. We present a new method that couples experimental small angle X-ray scattering techniques to detailed physics-based molecular simulation models to produce a powerful three-dimensional metrology for block-copolymer systems. As the method uses scattering techniques, it is able to provide statistical information over large regions, providing insight into long-range phenomena such as line edge roughness. We have used our simulation-based characterization technique on a variety of samples, all of which have shown excellent agreement with other, two-dimensional characterization techniques, such as scanning electron microscopy and atomic force microscopy.

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