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Examining the Self-Assembly of Rod-Coil Block Copolymers via Physics Based Polymer Models and Polarized X-Ray Scattering ADAM HANNON, DANIEL SUNDAY, DONALD WINDOVER, CHRISTOPHER LIMAN, National Institute of Standards and Technology, ALEC BOWEN, University of Chicago, GURDAMAN KHAIRA, Mentor Graphics, JUAN DE PABLO, University of Chicago, DEAN DELONGCHAMP, R. JOSEPH KLINE, National Institute of Standards and Technology — Photovoltaics, flexible electronics, and stimuli-responsive materials all require enhanced methodology to examine their nanoscale molecular orientation. The mechanical, electronic, optical, and transport properties of devices made from these materials are all a function of this orientation. The polymer chains in these materials are best modeled as semi-flexible to rigid rods. Characterizing the rigidity and molecular orientation of these polymers non-invasively is currently being pursued by using polarized resonant soft X-ray scattering (P-RSoXS). In this presentation, we show recent work on implementing such a characterization process using a rod-coil block copolymer system in the rigid-rod limit. We first demonstrate how we have used physics based models such as self-consistent field theory (SCFT) in non-polarized RSoXS work to fit scattering profiles for thin film coil-coil PS-*b*-PMMA block copolymer systems. We then show by using a wormlike chain partition function in the SCFT formulism to model the rigid-rod block, the methodology can be used there as well to extract the molecular orientation of the rod block from a simulated P-RSoXS experiment. The results from the work show the potential of the technique to extract thermodynamic and morphological sample information.

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