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MACHINE LEARNING AND DATA SCIENCE IN MATERIALS RESEARCH (MLDSMR) SEMINAR SERIES

Dr. Boran Ma
Assistant Professor
School of Polymer Science and Engineering
University of Southern Mississippi

Tuesday, November 5, 2024; 1 pm – 2 pm

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Meeting ID: 291 880 280 168
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Machine Learning-Aided High Throughput Examination of Block Copolymer Processing Conditions

Abstract: Block copolymer (BCP) thin films have a wide range of applications from membrane technologies for gas separation to energy applications including solid electrolytes. The nanoscale morphology of BCPs plays a critical role in the bulk material properties and subsequent applications. In addition to chemical structure, various processing conditions have been demonstrated to impact BCP morphology and can be leveraged as tunable parameters. To achieve precise control over BCP solid state morphology, processing conditions require optimization. This talk presents a novel approach for the high throughput analysis of grazing incidence small-angle x-ray scattering (GISAXS) data and atomic force microscopy (AFM) images, characterizing BCP thin film morphology. The curated dataset was used to train 11 unique machine learning (ML) models to predict BCP morphological properties from processing parameters including solvent ratio and additive amount. ML models were able to relatively accurately predict the extent of ordering of BCP thin films measured by GISAXS but struggled with AFM measurements. The decreased performance by the models predicting the AFM-based measurements can be attributed to the variability within the AFM measurements. Despite this variability, a convolutional neural network (CNN) trained on the AFM images was highly accurate, correctly classifying over 93% of images into ordered/disordered categories. While performance of ML models is crucial, interpretability of the predictions is equally important. For this purpose, the Shapley Additive exPlanations (SHAP) was used to interpret the predictions of the models. Additive amount was the most influential processing parameter on morphological output predictions, which agrees with the physical understanding of the system. Additionally, the SHAP deep explainer demonstrated the successful interpretation of the AFM images by the CNN. This framework leveraging ML and high throughput data analysis lays the foundation for BCP thin film processing optimization with an expanded design space.

Bio: Dr. Boran “Bo” Ma is an Assistant Professor in the School of Polymer Science and Engineering at the University of Southern Mississippi. Prior to joining SPSE in January 2023, Bo was a postdoctoral associate at Duke University. She received her PhD in Materials Science and Engineering from Northwestern University in 2019 and her BEng in Materials Science and Engineering from Harbin Institute of Technology in 2014. The Ma Research Lab focuses on multiscale modeling and simulation of polymeric materials and systems for energy and sustainability applications. Bo has been recognized as Early Career Researcher by ACS Applied Polymer Materials and MRS Communications. Bo performs stand-up comedy in her free time, and enjoys hiking, running, and paddle boarding.

For further information, please contact Dr. KT Tan at ktan@uakron.edu.