AI/ML/Autonomous Experimentation for Thin Films Processing

Room 317 - Session AIML1-FrM

Materials Design and Autonomous Discovery

Moderator: Eden Goodwin, Carleton University, Canada

8:15am **AIML1-FrM-1 Accelerating Discovery and Design for Thin Film Polymer Self-Assembly through Machine Learning***, Gregory Doerk,* Brookhaven National Laboratory **INVITED**

Thin film polymer self-assembly is a powerful approach to create nanoscale patterns across large areas with low cost for diverse applications in electronics and materials science. The confluence of compositional and architectural variation, entropic and surface energy constraints arising from thin film confinement, and process-dependent assembly pathways yields of panoply of nanoscale morphologies of which only a fraction can be discovered, catalogued, and engineered through manual experimentation. This talk will elaborate examples where artificial intelligence and machine learning (AI/ML) can accelerate thin film polymer self-assembly research. We describe the application of Gaussian process regression to automate x-ray scattering characterization for the discovery of new morphologies in template-directed self-assembly of block copolymer blends. We then illustrate the application of an active learning approach that incorporates foundation model-supported “few shot” image classification for determining processing-morphology relationships in spray-deposited block copolymer/homopolymer blend films using minimal quantities of data. Complementary in situ x-ray scattering measurements during spraying provide key mechanistic insights into trends in self-assembled structural organization across the process design space.

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