Abstract Submitted
for the DFD20 Meeting of
The American Physical Society

Data-driven analysis and prediction of multi-component polymer precipitation[1] PAVAN INGUVA, Massachusetts Institute of Technology MIT, LACHLAN MASON, INDRANIL PAN, MISELLE HENGARDI, OMAR MATAR, Imperial College London — The morphology of polymer blends can greatly impact material performance which consequently impacts the material choice and manufacturing processes. Characterizing the relationship between input parameters such as composition and thermodynamic interaction parameters, while desirable, is challenging due to the complex physics governing polymer blend precipitation which can be computationally expensive to solve numerically. To address this challenge, we present a workflow for integrating machine learning (ML) techniques to analyze and predict the output of physical simulations. We apply this workflow to study ternary polymer blends, however, it can be generalized to more complex systems. A set of ternary polymer blend morphologies is first generated using a modified multi-component Cahn-Hilliard model. The initial composition and material interaction parameters are varied. Subsequently, unsupervised ML is applied to cluster the simulation data, which is in the form of image data, into groups with distinct morphologies. With suitable cluster labels assigned to each data-point, a supervised ML algorithm can be employed to learn the non-linear relationship between the input parameters and the morphology which then enables the generation of predictive maps.

[1]This work is supported by the PREMIERE (EP/T000414/1) Programme Grant.

Pavan Inguva
Massachusetts Institute of Technology MIT

Date submitted: 29 Jul 2020 Electronic form version 1.4