Advances and Challenges in Numerical Studies of Polymeric Systems

*Su-Mi Hur+, Juhae Park, Jihun Ahn, Vikram Thapar
School of Polymer Science and Engineering, Chonnam National University, Gwangju 61186, Republic of Korea
+E-mail: shur@jnu.ac.kr

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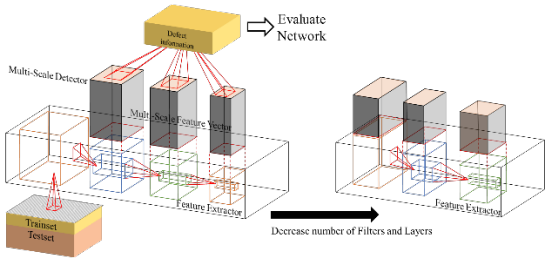
1. Introduction

Various theoretical and numerical approaches have provided valuable insights into understanding the underlying physical principles in various polymeric systems and powerful tools and guidelines for designing experiments [1]. However, often complicated interactions, and a wide range of length and time scales related to self-assembled structures in polymeris systems prevent the usages of existing theoretical/numerical models which only applicable in limited cases. Our recent efforts on overcoming the limitation of existing models and extending the scope of numerical approaches including deep learning will be introduced in this presentation [2,3].

2. Numerical Methods

2.1 Deep Leaning: Recently deep learning has proven its potential in various research fields and has become one of the most attractive tools. There have been attempts to apply deep learning in designing molecules structures, analyzing spectral data, and even sampling more accurate free energy landscapes. We develop a deep learning algorithm which modifies YOLOv3 (you only look once) model to detect and classify defects in scanning electron microscopy (SEM) images featuring self-assembled line-space patterns in block copolymer thin films.

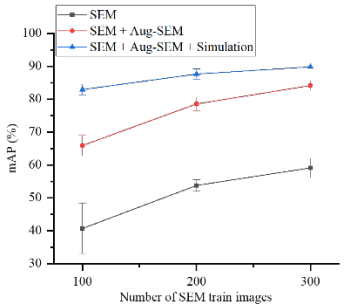


2.2 Coarse-Grained Simulation Model: We propose an efficient coarse-grained model which allows predict the morphology of amphiphilic system over a wide range of concentrations and solvent qualities. To prepare a simulation dataset for deep learning, we use theoretically informed coarse-grained model (TICG) combined with Monte Carlo simulations. That model has been rigorously studied and validated with available experimental data for copolymer thin films.

3. Results and Discussion

Developed numerical model predicts the self-assembly of amphiphilic block copolymers under the various solvent and confinement conditions. Model parameters are directed mapped to solvent quality and interfacial tensions of the systems through scaling analysis of single-chain size and molecular dynamic simulations.

The network performance which is poor with a small training dataset of the real SEM data (100 images), has been greatly enhanced with the use of data augmentation strategies; namely flipping of images and mixing of images with images collected from theoretically informed coarse-grained simulations. Further improvements were earned by increasing the percentage of real data in training set, whereas benefit achieved by augmentation was more predominant when number of real images was smaller.



4. Conclusions

The coarse-grained model of generalized Hamiltonian captures non-flat free surface (soft confinement) driven self-assembly and allows predicting the self-assembly of amphiphilic polymeric system over a wide range of concentrations and solvent qualities. Applying machine learning to material science fields has been also explored. Modified YOLOv3 is applied to detect and classify defects. To ensure the satisfactory performance of the network under the constraint of lack of available data, we optimized the network's architecture and employed the two strategies of data augmentation.

References

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[3] J Ahn et al., *Journal of Micro/Nanopatterning, Materials, and Metrology*, 20(4), 041202, 2021

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