Segregation kinetics and applications of brush-modified surfaces

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by
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Chapter 6

Summary and future plan

6.1 Summary

In this chapter, we briefly summarized our work so far. Chapter 1 details the phase separation kinetics and its application in enzyme adsorption and oil-in-water via brush-modified surfaces. In Chapter 2, we have successfully developed a versatile and reliable simulation model for the surface fabrication of MPs in various shapes, such as cups, spheres, and flat (rectangular/disc-shaped) MPs, with surface-initiated ATRP brush grafting. Our observations show that there is an increase in biopolymer adsorption with the following factors: (i) brush length, (ii) initiator concentration, (iii) biopolymer concentration, and (iv) biopolymer size. Furthermore, we found that at late times, the flat surface (rectangular/disc-shaped) could adsorb more biopolymers than the other two surfaces we studied. Additionally, we have demonstrated that longer biopolymer chains lead to significantly higher biopolymer loading for all surfaces. In Chapter 3 of our analysis, we found that JPs with lower initiator concentrations had longer brush lengths, which supported more stable emulsion formation by preventing oil clustering compared to shorter chains. Similarly, when we looked at JPs with different initiator concentrations but kept the length of grafted polymer brushes constant by adjusting the monomer conversion, we noticed surface modification with varying local grafting brush densities. Higher initiator concentrations led to increased grafting density and vice versa. We observed more stable emulsions with JPs having high brush density. When we kept the initiator concentration constant and varied the length of polymer brushes, we found that longer brushes led to more stable emulsions. In Chapter 4, an extension of our previous work, we analyzed the emulsion stability and found that TP-1 > TP-4 (lower c_i) and TP-3 > TP-2 (higher c_i). We also observed increased stable emulsion formation by increasing the brush densities for TP-1, TP-3, and TP-4. Our simulation results align with experimental findings. In Chapter 5, we studied the impact of disorder on segregation kinetics. We found that during a deep quench, lower levels of disorder had almost negligible impact. When the quench was shallow, and disorder levels were low, the scaling functions deviated slightly as the system evolved to form fragmented lamellar stripes. With a high level of disorder, lamellar patterns eventually formed at all quench depths. We also observed a crossover in the length scale for a high level of disorder, which stabilized at later times. Additionally, the morphologies aligned in the direction of a higher number of disorder sites on the lattice.

6.2 Future plan

Currently, I am continuing with three projects: one is Self-assembly of charged/uncharged nanorods in phase-separating fluids under the effect of photo-controlled reactions.

The study on the Effect of photo-controlled reactions on Self-assembly of charged/uncharged nanorods in phase-separating fluids. This study has several important implications in the field of nanotechnology. Self-assembly is a critical process in the design and synthesis of functional nanomaterials. It can lead to novel nanostructures with unique physical properties. Understanding the factors that influence the self-assembly of nanorods is crucial for developing new materials with tailored properties for various applications, such as sensors, electronics, and energy conversion devices. Furthermore, studying the effect of photo-controlled reactions on the self-assembly of nanorods can open up new possibilities for the dynamic control of

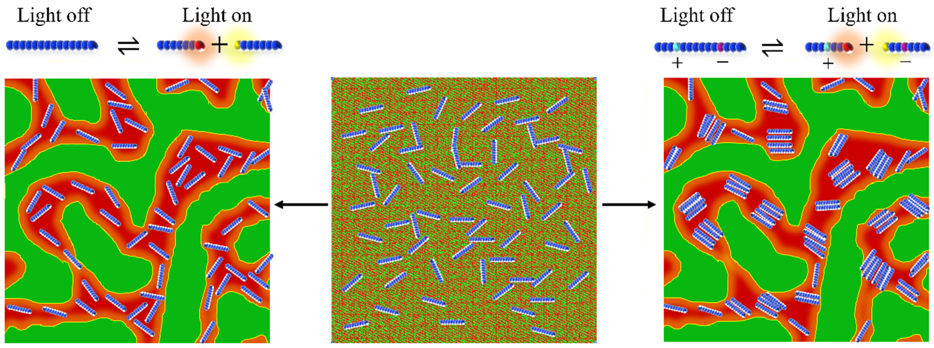

Fig. 6.1: Schematic of our simulation study on the self-assembly of nanorods in polymer matrices or binary fluid mixtures. We will utilize DPD and MD simulation techniques. In this work, we first report on the self-assembly and phase behavior of photo-sensitive nanorods in multicomponent fluids to evaluate the role of entropic and enthalpic factors that control the aggregation/dispersion process of nanorods. Second, we study the self-assembly of electrically charged photo-sensitive nanorods in phase-separating fluids. Next, we assess the effect of nanorods on the evolution morphology, growth law, and scaling phenomena in such systems.

nanomaterials. Photo-controlled reactions in these systems allow for precise and reversible manipulation of the assembly process, providing a way to tune the properties of the resulting materials on demand. This could lead to the development of smart nanomaterials that respond to external stimuli, such as light, for use in advanced sensing or drug delivery applications.

Further, electrostatic charge and chain length are other key parameters that affect the self-assembly of nanorods. Understanding how these factors influence the assembly process can help optimize the design of nanorod-based materials. For example, controlling the electrostatic interactions and chain length could create new self-assembled structures with specific properties.

This work can play a valuable role in understanding the unique process of developing arrested morphologies by controlling the combined process of phase separation, polymerization, and crosslinking of nanorods mimicking rigid proteins such as β-keratin. To the best of our knowledge, developing a frozen morphology using phase separation and polymerization has not yet been studied adequately. Motivated by this, we aim to design a robust computational model by adapting our recently developed DPD simulation approach for controlled polymerization so that it can capture the essential features of β-keratin gel formation, such as (i) the distribution of the β-keratin chain length, (ii) time evolution of the gel network. Furthermore, we will study the effect of varying the crosslinker concentration and polymerization reaction rates on the material's structural properties and the phase separation process that leads to forming materials with various arrested morphologies.

The second one is the Segregation kinetics of cyclic amphiphilic diblock copolymers via DPD simulation. The third one is a DPD simulation study on the segregation kinetics of dimers in solution.