

DISSIPATIVE PARTICLE DYNAMICS IN SOFT MATTER AND POLYMERIC APPLICATIONS — A REVIEW

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Computer simulations and in particular mesoscopic simulation techniques such as the dissipative particle dynamics (DPD) technique, enable researchers to study the complexities of soft material and polymeric systems by performing *in silico* experimentations alongside *in vivo* experiments. In addition, these mesoscopic simulations allow scientists and engineers to characterize and optimize the actual experiments in a more efficient manner. The DPD is one the most reliable mesoscopic simulation techniques for phenomenological investigation of soft matter and polymeric systems. In this review, which is complimentary to an earlier review also by the present authors on DPD methodology and complex fluid application (Moeendarbary *et al.*, 2009), we categorize and review the notable published works, and document efforts that applied the DPD simulation technique to various important soft matter and polymeric applications, over the last decade.

Keywords: DPD review; DPD application; mesoscopic simulation; soft matter; polymeric system; DNA migration; Self-assembling; polymer drop/brush; block polymer; Micelles formation; lipid bilayer; system of surfactants/amphiphiles.

1. Introduction

Soft matter and polymeric systems, in which the macroscopic properties and observable behaviors have significant dependency on the microscopic structures, can include a variety of structures such as solutions or melts of polymers/gels, mixtures of biological membranes/micelles/vesicles, etc. There exist broad applications of such systems in industrial technologies (lubricants, oil recovery, plastics, liquid crystals, and paints) and especially in the field of biological and biomedical sciences (biochemical lab on chip systems, separation devices and drug delivery systems). Over the last few decades, there have been notable experimental, theoretical and computer modeling research methodologies applied for the interpretation of physical properties of such systems. However, due to complexity and interplay of several time and length scales, a unified theoretical basis for the understanding

of soft matter systems is difficult. Conducting actual experiments are always helpful to obtain insights into the various phenomena occurring in these systems. Still, these experimental approaches are usually very costly, time consuming and require significant efforts. Computer simulation is an alternative way to visualize, characterize, and optimize different features and designs of these complex systems. Recently, due to the rapid advancements of computing hardware, facilitating higher computational speeds and larger storage and/or memory capacities, numerical modeling and simulation is becoming a powerful and acceptable methodology for investigating the static and dynamic properties of soft matter and polymeric systems with varying space and time scales.

In order to perform computer modeling for soft matter and polymeric systems, robust and accurate techniques are essential since the occurrence of the physical phenomena of interest in such systems can range from the nanoscale to macroscopic scales. Furthermore, there may exist features of coupled electrical, mechanical, thermal, and fluid domains, as well as geometrical complexities in certain applications. In general there are three methods for the simulation of such systems, namely: molecular dynamics (MD), continuum methods (Navier-Stokes) and mesoscopic methods, and each of these have their own characteristics, advantages and disadvantages. At the macroscopic scale, a simple fluid can be described by continuum Navier-Stokes equations and sophisticated computational and numerical discretization techniques have been developed over the years for the solution of these differential equations. These discretization methods are usually based on conventional finite-differences, finite-elements, finite-volumes, or they can rely on some more robust techniques, such as spectral-elements (higher order finite-elements), meshfree methods and the force coupling method, each of which are appropriate for different applications. These continuum approaches are able to capture the hydrodynamic behaviors well at the macroscale. However, these methods are based on natural constitutive equations which capture the microscopic details of the fluid in a phenomenological manner, and as a result are not suitable for many soft matter applications, Marsh [1998].

On a microscopic level, and up to a few nanometers in length, and a few nanoseconds in time, the MD and Monte Carlo (MC) methods enable relatively accurate simulation of very small volumes of liquid. Following the position and the momentum of every atom/molecule, MD can deal effectively with nano-domains and is perhaps the only accurate approach in simulating flows involving very high shear where the continuum or the Newtonian hypothesis break down. More specifically, for dimensions less than around ten molecules, the continuum hypothesis breaks down for liquids, and MD should be employed to simulate the atomistic behavior of such systems, Karniadakis *et al.* [2005]. Although microscopic approaches have become increasingly successful in the simulation of a small number of atoms/molecules, it is not easy to apply these techniques to large complex systems and it would incur huge computational costs to reach time-scales over which hydrodynamic effects are significant.

One of the main objectives in mesoscopic simulations is to identify characteristic physical lengths and times in the system, which are then used to simplify

complex models. For example, in polymeric systems, the hydrodynamic behaviours are easily modeled using continuum techniques but it is expensive to handle them at atomistic levels. On the other hand, the interaction between components at the atomistic scale can be taken into account by employing molecular methods, and these atomistic features are very difficult, if not impossible, to capture through continuum methods. The development of intermediate techniques, which possess both features of micro- and macro-scales methods, are thus essential. Depending on the nature of the application, several mesoscopic simulation methods have been devised, developed and refined over the years. For the polymeric systems, some of the intermediate techniques include Brownian dynamics (BD), dissipative particle dynamics (DPD), lattice Boltzmann (LB), time-dependent Ginzburg-Landau (TDGL) method and the dynamic density functional theory (dynamic DFT) method, please see the review of Zeng *et al.* [2008] for more information on these techniques. The dissipative particle dynamics (DPD) technique is an alternative method for mesoscopic soft matter simulation, which was first devised and developed for simulating hydrodynamic behaviour by Hoogerbrugge and Koelman [1992] and Koelman and Hoogerbrugge [1993]. It was subsequently modified by Español and Warren [1995]. This method can be perceived as the clustering a number of molecules into single particle where the number of molecules per DPD particle is known as the coarse-graining parameter [Español *et al.*, 1997; Flekkøy and Coveney, 1999; Flekkøy *et al.*, 2000; Kinjo and Hyodo, 2007].

The aim of this review is to document the most representative works which employ the DPD technique in soft matter and polymeric applications. In the next section, we provide a comprehensive review of DPD applications in soft matter and polymeric systems including macromolecules and polymer drops, block copolymers, membranes, and grafted polymer brushes. Subsequently in section 3, we look at some of the recent advances in modeling surfactant and amphiphile systems through DPD simulations.

2. Polymeric Systems

The configurational and dynamical behaviours of polymers typically occur at mesoscopic time- and length- scales, thus enabling the DPD bead-spring representation of polymers. This results in an ideal tool for studying and understanding the rheological properties of polymeric systems. Moreover, in DPD polymeric systems, the solvent particles are explicitly accounted for through unconnected DPD particles and this leads to more realistic simulation results compared to conventional theories for polymer solutions.

2.1. Rheological properties of polymers

Both hydrodynamic interactions and excluded volume effects are naturally taken into account in the DPD model for polymers, and consistent results have been

obtained for the scaling laws, [Schlijper *et al.*, 1995; Zhang and Manke, 2000b]. Kong *et al.* [1994] are probably the earliest authors who had studied the effects of polymers confined between parallel walls via the DPD technique. The associated shear thinning and normal stress effects were subsequently studied, [Kong *et al.*, 1997b; Schlijper *et al.*, 1997]. Kong *et al.* [1997a] further investigated the influences of solvent quality by varying the repulsive interactions between particles. In this work, the scaling exponents for the radius of gyration of polymers in dilute solution of different solvent quality was found to vary in reasonable fashion and the calculated relaxation time confirmed the Zimm theory Kong *et al.* [1997a]. Comparable DPD results were obtained more recently for scaling exponent, Ilnytskyi and Holovatch [2007], and for different levels of coarse-graining [Guerrault *et al.*, 2004; Kindt and Briels, 2005].

In addition to the proper reproduction of scaling exponent for self-avoiding chains, the DPD simulations of polymer melt by Spenley [2000] showed excellent agreement with the Rouse model. DPD simulations of dilute polymer solutions under shear flow and shear thinning effects were reported by Pan and Manke [2002]. DPD simulation of the pressure driven flow enabled Willemsen *et al.* [2002] to study the conformational behaviour of polymer chains within a square capillary. In the Rouse model, chain segments are free to cross each other. Thus, in order to simulate the polymer entanglement accurately and reduce the frequency of artificial chain segment crossing, Pan and Manke [2003] introduced a segmental repulsion algorithm. For scaling of viscosity and centre of mass diffusion coefficients, transitions in scaling exponents at a critical entanglement chain length were observed in their DPD simulations Pan and Manke [2003].

More recently, Nikunen *et al.* [2007] introduced a simple and computationally efficient criterion based on a simple geometrical argument for chain crossing avoidance. They applied their model in DPD simulations of linear melt of homopolymers and achieved Rouse dynamics for short chains and reptational dynamics for longer chains. The Rouse and reptational dynamics were observed in DPD simulations of the diffusion of a strongly adsorbed polymer chain on a solid surface in dilute solutions by Qian *et al.* [2007]. In addition, it was found that the interactions between the surface and the fluid screen the hydrodynamic interaction. Under typical DPD simulation conditions, Jiang *et al.* [2007] found that the Zimm model is obeyed for polymer dynamics in dilute solution, exhibiting reasonable capturing of hydrodynamic and excluded volume interactions. However, in lower Schmidt number regimes the Rouse dynamics was found to be dominant.

2.1.1. *Macromolecular and DNA migration*

Recently, there have been a lot of attention in macromolecular transport in micro/nano channels due to the wide variety of applications in chromatography and electrophoresis separation devices. The existence of complex geometries and coupling of fluid flow with other external force fields in these applications make the

DPD one of the best alternative direct simulation techniques to study the dynamical behaviours of these systems. Using a DPD model of finitely extendable nonlinear elastic (FENE) chain, Fan *et al.* [2003] were able to fit the velocity profiles of FENE chain suspensions with power-law curves. The DPD results of the wormlike chain under shear flow were found to match well with the single DNA experiments by Symeonidis *et al.* [2005]. Later, Fan *et al.* [2006] studied flows of a DNA suspension through microchannels by employing DPD simulations of the wormlike chain.

Millan *et al.* [2007] studied the effects of bead number, polymer concentration, and flow rate on the streaming of polymer solution in pressure driven flow. In their DPD simulations, the highly anisotropic and nonuniform distribution of polymer conformation was observed and it was found that short chains tend to migrate away from the walls of the channel while for long polymers, movements toward the walls was favoured. He *et al.* [2007], using two dimensional DPD simulations, explored the effects of field strength, chain length, solvent quality and pore size on the translocation of a single polymer chain through a pore under a fluid field.

2.1.2. Viscoelastic flow and dynamics of polymer drop

Providing a model for viscoelastic flow, Ten Bosch [1999] introduced the spring elasticity to each DPD particle, and through this, Ellero *et al.* [2003] devised the viscoelastic version of the finite point method (FPM). Chen *et al.* [2004] investigated the dynamics of polymer drops, consisting of a mixture of DPD solvent particles and FENE bead spring chains, under steady-state and transient shear flow in a microchannel. The shear thinning and normal stress difference effects were observed, and in a steady shear field, the relation between deformation parameter and capillary number were described into linear and non-linear regimes. A sufficiently elongated drop under high shear rate will break up while possible coalescence may occur for two neighbouring drops. Moreover a tumbling mode was observed for polymer drops at high Schmidt numbers. Using DPD and selecting different initial geometries of the ellipsoids, the process of ellipsoidal drop retracting was simulated by Liu *et al.* [2004, 2005] in order to measure the interfacial tension between two immiscible polymers. Heine *et al.* [2003] employed molecular dynamics simulations to study the spreading dynamics of polymer droplets and they also evaluated different implementations of the Langevin and DPD thermostats for efficiency and practicality in preserving the hydrodynamic effects. Somfai *et al.* [2006] connected DPD particles to form dumb-bells and they believed that this could be the initial steps for further establishment of a new model to study instabilities and turbulence in viscoelastic fluids apart from conventional models that have the high Weissenberg number problem. In an attempt to probe some of the viscoelastic behaviours of filled rubbers, Raos *et al.* [2006] conducted DPD simulations and they found that particle-particle interactions have notable effect on the in-phase component of the dynamics shear modulus and also may be responsible for some strain dependence of the modulus. Employing the DPD technique to describe relaxation mechanisms in

soft thermoplastic elastomers, Long and Sotta [2006, 2007] proposed a model consisting of hard spheres embedded in an elastic matrix. The response of the thermo plastic or filled elastomers to different kind of deformations was examined and the elastic and plastic regimes of deformation were subsequently characterized, Long and Sotta [2006].

2.2. Block copolymers and mesophase separation

One of the most fascinating subjects in polymer melts is the formation of block copolymers which consist of multiple blocks (usually two) of polymers that are chemically connected from end-to-end. Under different conditions of temperature, length-ratio of the blocks, concentration and structure of the block copolymers and according to their aggregation structure, they are able to form micelle, biocontinuous, hexagonal and lamellar phases Cao *et al.* [2005]. From DPD simulations of soft sphere strings, it was found that instead of macrophase separation, microphase separated structures are formed when a melt of these polymers are quenched Groot and Madden [1998]. Transition of a copolymer system from one mesophase structure into another is an important phenomenon, and the DPD method is proving to be a promising technique for predicting the dynamical pathways and formation of copolymers following a temperature quench till the system reaches equilibrium Groot and Madden [1998].

In the following discussion, we review several publications which use the DPD technique to examine morphology and phase separation of these melts of various structures under different conditions. The first fundamental DPD simulation of copolymers is the work of Groot and Madden [1998] where the mesophase formation of linear ($A_m B_m$) diblock copolymer melts was studied. Depending on the length ratio of the two blocks and the Flory-Huggins χ -parameter, the polymer melts, in which chains are represented by the short strings of soft DPD particles connected by harmonic springs, form mesoscopically ordered structures. The order of equilibrium structures changes to lamellar, perforated lamellar, hexagonal rods and micelles as the polymer becomes more asymmetric, and the simulations showed that the hexagonally perforated lamellar stable phase corresponds to the prediction of the gyroid phase in the mean-field theory.

Depending on the volume fraction of the end blocks f_A , similar morphologies were observed for the self-assembly of symmetric triblock copolymers (ABA) by Abu-Sharkh and Alsunaidi [2006]. Also Yang *et al.* [2005] used a Monte Carlo scheme to calculate the Flory-Huggins parameter χ required in mesoscale DPD investigation of miscibility and morphology of different polymer blend mixtures. In Groot and Madden [1998], the authors observed the formation of a series of metastable phases through a nontrivial pathway before equilibrium is reached. For the evolution of the mesophases, they found that either hydrodynamic interactions or the precise form of the Onsager kinetic coefficient to be important. More detailed simulations of the gyroid phase were performed more recently by Martínez-Veracoechea and

Escobedo [2006] for pure diblock copolymers and using two different mesoscopic models (Monte Carlo and DPD) and the gyroid phase and nodal chain stretching were duly observed.

The next central work in this area is that of Groot *et al.* [1999] who studied the role of hydrodynamic interactions in microphase formation by performing DPD simulations that can capture correct hydrodynamic forces of the melt, and comparing the data with that of Brownian dynamics (BD) simulations. For the evolution of asymmetric block copolymers, the lack of hydrodynamic interactions in the BD simulations leads to the melt remaining in a metastable phase and failing to reach the correct equilibrium state obtained by DPD simulations, which is also predictable by the mean-field theory. However, because the hexagonal phase forms via a metastable gyroid-like structure while the lamellar phase is formed via spinodal decomposition, in the evolution of symmetric block copolymers the hydrodynamics seems to be unimportant. On the other hand, Horsch *et al.* [2004] studied the hydrodynamic effects in the structure of diblock copolymer melts using BD, molecular dynamics and DPD simulations, and they obtained the hexagonal ordered cylinder phase when using BD simulation.

AlSunaidi *et al.* [2004] studied the liquid-crystalline ordering in rod-coil diblock copolymers. The application of DPD to anisotropic media and to the field of computational rheology of liquid crystals was reported in Bras *et al.* [2005], Gomes *et al.* [2005] and Levine *et al.* [2005] and the nematic and smectic mesophases were simulated by Levine *et al.* [2005]. Qian *et al.* [2005b] employed DPD to explore the effects of adding block copolymers to immiscible binary system of same homopolymer blends and they found increasing copolymer (especially shorter block copolymer chains) concentration, resulting in reduction of interfacial tension. Subsequently, the structural properties and arrangement of the immiscible polymer blends in a system consisting of their diblock copolymer was studied by Travis *et al.* [2007]. To obtain molecular details of polymer nanocomposites, Liu and Zhong [2006] studied the self-assembly of binary nanoparticle mixtures in lamellar diblock copolymers. Later, Huang and Wang [2007] included DPD solvent particles to study the aggregation behaviours of nanoparticles in ternary systems and in applications of biomimetic mineralization. Depending on the volume fraction of double-hydrophilic block copolymer, the aggregation process evolved from one large aggregate to other various ordered nanostructures like dispersed aggregates, hexagonally packed cylinders, and lamellae.

From the DPD simulations of Qian *et al.* [2005a], microphase separation of cyclic block copolymer ($c-A_mB_m$), which is similar to the linear block copolymer but has no chain ends, showed similar phase diagram of the linear block copolymer. You *et al.* [2007] investigated the microphase transition of perforated lamellae cyclic diblock copolymers under steady shear, while Cao *et al.* [2005] observed the influence of architecture and concentration on the shape and size of block copolymers by DPD simulation of aggregation of three block copolymers with the same composition but

different architecture in aqueous solution. They found more extendable morphologies for di- or tri-block copolymers with hydrophilic ends compared with triblock copolymer of hydrophobic ends.

To test the effects of the molecule rigidity, Qian *et al.* [2006a, 2006b] introduced a bond angle potential in their DPD model of $A_2(B_4)_2$ -type miktoarm, and they found that the increase of the stiffness of the B arms enabled the randomly distributed spheres to be packed into an ordered BCC array and they also observed a hexagonal cylindrical and a parallel ellipsoid in lamellae structures. Following this and by varying the composition and interaction parameter, the systematic phase behaviour for of AB_2 miktoarm star copolymers was constructed by Huang and Yu [2007] via DPD simulation, and it was shown that in order to reduce the contact level between A and B , the A and B arms tend to separate from each other, and the two B arms are squeezed onto the same side.

DPD studies for the morphologies of linear and graft fluorinated pure block copolymers and also their incorporation with solvent molecules were reported by Özen *et al.* [2006]. Subsequently, Huang and co-workers [Huang and Chen, 2007; Huang and Lin, 2007] investigated the self-assembling behaviours of A_2 -star- $(B$ -alt- $C)$ and A -block- $(B$ -graft- $C)$. Please see Fig. 1 for the schematic of the block copolymers, while for the first molecule, some of the morphologies are shown in Fig. 2.

Xu *et al.* [2006b] reported the microphase separation of star diblock copolymer melts; they employed a Gaussian chain model to describe two types of $(A)_4(B)_4$ and $(AB)_4$ star diblock copolymers which are constructed by joining four identical linear diblock copolymers. They found similar ordered mesostructures as those of corresponding linear and cyclic ones, and they further observed that microphase separation activated more easily for $(A)_n(B)_n$ than corresponding $(AB)_n$ under similar conditions. Subsequently, Soto-Figueroa *et al.* [2007] simulated linear and 3-arm ploy(styrene)-ploy(isoprene) block copolymers while employing DPD combined with Gaussian models and their simulations predicted well the microphase separation, order-disorder transition, and self-assembly of the ordered structures with specific morphologies such as body-centred-cubic (BCC), hexagonal packed

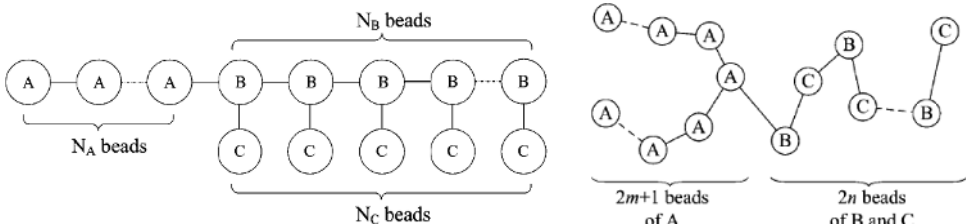


Fig. 1. Schematic diagram of Left: A -block- $(B$ -graft- $C)$, Right: A_2 -star- $(B$ -alt- $C)$. [Huang and Chen, 2007; Huang and Lin, 2007], Copyright Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.

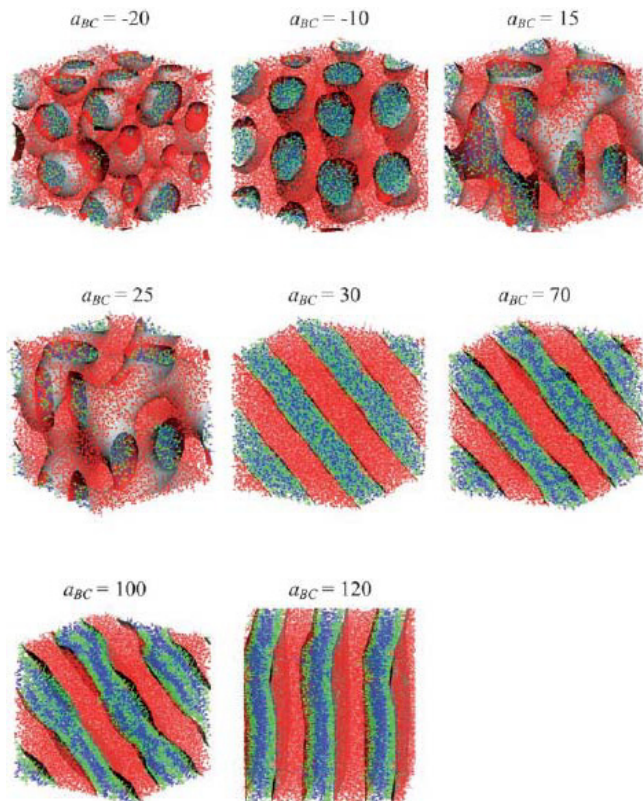


Fig. 2. Morphology variation of A_2 -star-(B -alt- C) copolymers with a_{BC} (repulsion parameter). The red, green, and blue colours represent A , B , and C , respectively. The red surface corresponds to the iso-surface of component A . Huang and Chen [2007], Copyright Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.

cylinders (HPC), hexagonal perforated layers (HPL), alternating lamellar (LAM), and ordered bicontinuous double diamond (OBDD) phases.

2.2.1. Effects of steady shear

In Zhang and Manke [2000a], the morphologies and flow-induced microstructural transitions of diblock copolymer melts under the steady shear flow (which is generated using Lees-Edward boundary condition) is investigated and they observed from the prediction of rheological properties a strong enhancement in viscosity and first normal stress coefficient for the body-centre cubic (BCC) spherical equilibrium microstructure relative to the disordered system. Similarly and under steady shear condition, the microphase separation, end-to-end distance and shear viscosity of linear dendritic diblock copolymers were investigated by Liu and Zhong [2005] using DPD simulations and it was observed that both the shear rate and the degree of branching play important roles in microstructure and properties, that can lead to

new materials for new applications. Morphology changes and alignment of lamellar diblock copolymer under steady shear were examined using DPD by Liu *et al.* [2006] and Lísal and Brennan [2007], and more recently Lísal and Brennan [2007] found that at low shear rates, the parallel lamellar orientation which has higher internal energy is preferable while the perpendicular structure which has higher entropy production is favourable at high shear rates.

2.2.2. *Micelles formation*

Formation of micelles, and more specifically multicompartment micelles, from block copolymers, which finds new applications in the field of drug delivery, and their morphology and rheology in different shapes and solutions is another favourable area in which DPD simulations can be exploited, [Chou *et al.*, 2006; Cui *et al.*, 2006; Xia and Zhong, 2006a, 2006b; Liu and Zhong, 2007; Sheng *et al.*, 2007; Xia *et al.*, 2007; Xia and Zhong, 2007; Xin *et al.*, 2007; Zhong and Liu, 2007]. In Cui *et al.* [2006], the rheological occurrence of shear thickening and thinning in the solution of these micelles under shear was observed. Through DPD simulations, Xia and Zhong [2006b] demonstrated that a multicompartment micelle could store two or more agents within separate nanoscopic compartments simultaneously, and the distributions of the agents can be tailored by changing the interactions between incompatible species.

In Xia and Zhong [2006a], the formation of multicompartment micelles from *ABC* star triblock copolymers was studied. Later, the effects of architecture, block length, and solution concentration on morphologies of both star and linear triblock copolymers in aqueous solution was examined by Chou *et al.* [2006], Xin *et al.* [2007] and Zhong and Liu [2007], and these works were extended for morphologies of two-compartment micelles formation of linear pentablock copolymers by Liu and Zhong [2007]. Also, Sheng *et al.* [2007] investigated the micellization of diblock copolymer in dilute solution and the influence of the compatibility between blocks. Similarly and in a condition of dilute solution, morphologies of star block copolymers was explored by Sheng *et al.* [2006] and it was found that the tendency of forming micelle and the supramolecular structures is different between the $(AB)_n$ and $(BA)_n$ types. Subsequently, multicompartment micelle formation from π -shaped *ABC* block copolymer was observed by Xia and Zhong [2007] and the creation of oblate and trumpet vesicles was reported by Xia *et al.* [2007].

2.2.3. *Effects of confinement*

Xu *et al.* [2006a] employed DPD to investigate the mesoscale structure of symmetric diblock copolymer confined in a cylindrical tube and following this, Feng *et al.* [2006] found that the morphology of this confinement depends on the volume ratio of the immiscible blocks, the diameter of the cylindrical tube and the interactions between the blocks, and between the wall and blocks. Similarly and more recently,

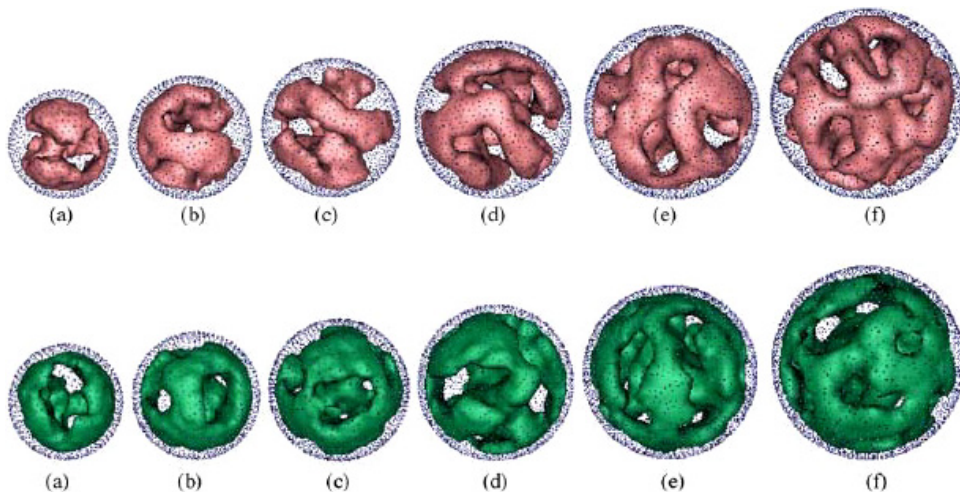


Fig. 3. Morphologies of A5B5 in spherical nanodroplets with neutral (top) and non-neutral (Bottom) surface. Radius of sphere: (a) 5, (b) 6, (c) 7, (d) 8, (e) 9 and (f) 10. Reprinted from Feng *et al.* [2007], Copyright (2007), with permission from Elsevier.

morphologies of diblock copolymer in a nanospheres of different sizes and different interfacial energies were studied by Feng *et al.* [2007], see Fig. 3.

2.3. Membrane morphology and formation of lipid bilayer

The hydrophobic tail and a hydrophilic head of amphiphilic molecules aggregate into several structures, as some of these structures such as the spherical micelles and rod like or spheroidal micelles were investigated by DPD simulations as discussed in previous sections. More importantly these amphiphilic systems can form bilayer membranes and vesicle (liposomes) structures which are the critical components of all biological membranes that protect and detach cells from their surroundings. The structures of these membranes consist of nanometre order of magnitude thicknesses combined with micrometer area dimensions such that the usual microscopic or macroscopic simulation models are not able to mimic the complete structures. In addition, the time scales involved in the evolution of these assemblies span from atomic to macroscopic lengths and therefore only mesoscopic techniques such as the DPD method can handle the dynamics of such systems. For a full review, please see Shillcock and Lipowsky [2006] and Venturoli *et al.* [2006]. Moreover DPD enables the study of mesoscopic cellular phenomena hundreds of times faster when compared with MD simulations.

The first attempt of the use of DPD simulation in biological membranes was made by Groot and Rabone [2001] who employed the method to reproduce the phosphatidylethanolamine membrane structure and to determine the rupture properties of its mixed bilayers. In their simulations, and during the study of the diffusion of water through the mixed bilayers of lipid and non-ionic surfactant, the formation

of small holes was observed at different surfactant concentrations. The DPD simulations of Shillcock and Lipowsky [2002] demonstrated that under certain concentration and amphiphile structure, the planar bilayers were created from amphiphiles even without the existence of attractive forces, and in order to form the natural structure of lipid membrane, strong chain stiffness potential was found to be vital. Additionally, in Shillcock and Lipowsky [2002] and Sugii *et al.* [2007], DPD simulations were used to measure surface tension of the bilayers and estimated bending rigidity showed agreeable results compared with other reported experimental and numerical results. Jakobsen *et al.* [2005] reported that mechanical and diffusional properties of a lipid bilayer membrane in its fluid phase become altered by the action of phospholipase A_2 .

In Ayton and Voth [2002], the DPD method was recast in an elastic membrane formulation to construct the elastic membrane DPD (EM-DPD) model by which the dimyristoylphosphatidylcholine bilayer at high and low surface tensions was studied. Later in Li *et al.* [2004], the bond angle potential model was added in DPD simulations of the inverted phase of a lipid to achieve the correct elastic properties of the membrane. In order to calibrate the DPD parameters for the system of membrane patches of diblock copolymers of various molecular weights, Ortiz *et al.* [2005] used data obtained from atomistic MD simulations. Lipidic membrane fusion was studied by Li and Liu [2005] where DPD results were compared with continuum elastic models. More recently, Gao *et al.* [2007] achieved less stretchable bilayers in DPD simulations based on a new parameterization of repulsive interactions.

Kranenburg *et al.* [2003a, 2003b] carried out DPD simulations to study complex phase behaviour of phospholipid bilayers. In order to reproduce the natural state of a tensionless bilayer, DPD was combined with a Monte Carlo scheme and the influence of surfactant structure and temperature on bilayer thickness and the orientational order parameters were investigated. In addition, for single/double-tail surfactants, the conditions that induce a gel interdigitated phase in the bilayer was investigated. Later Kranenburg and Smit [2004] and Kranenburg *et al.* [2004] added alcohol molecules in their system of water and double-tail lipids to study the induced interdigitation of bilayers. They found that the addition of alcohol molecules screens the hydrophobic tails from the water phase so that the normal bilayer structure changes into a monolayer, see Fig. 4.

The spontaneous formation of vesicle, from both a randomly dispersed system and a bilayer structure of amphiphiles in water particles was studied by Yamamoto *et al.* [2002], where DPD simulations confirmed that during the vesicle formation process, the hydrophobic interaction energy is minimized and the two-tailed amphiphiles aggregation is also much faster than single-tailed models. By means of DPD simulations, Laradji and Kumar [2004, 2005] found that the area to volume constraint has a high impact on the system pathway between the regimes corresponding to coalescence of flat patches, budding and vesiculation, and coalescence of caps. Shillcock and Lipowsky [2005] and Grafmüller *et al.* [2007] performed

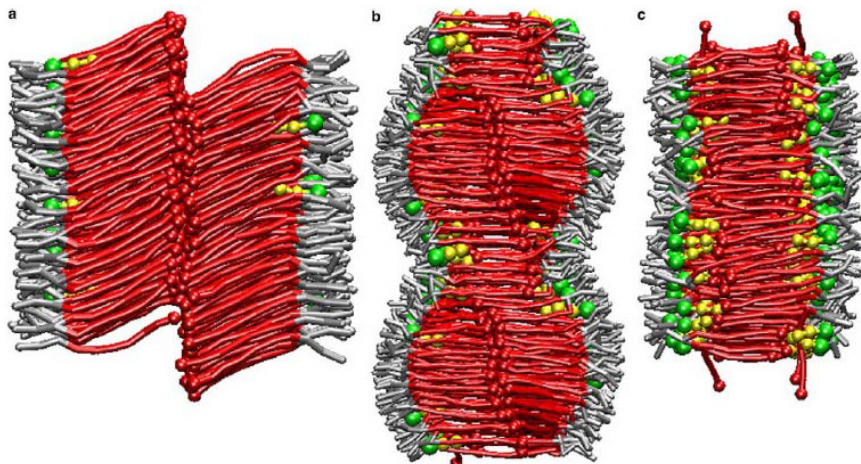


Fig. 4. Snapshots of a bilayer consisting of the lipid $h_3(t_7)_2$ with various concentrations of the model alcohol ht_2 . Reprinted from Kranenburg *et al.* [2004], Copyright (2004), with permission from Elsevier.

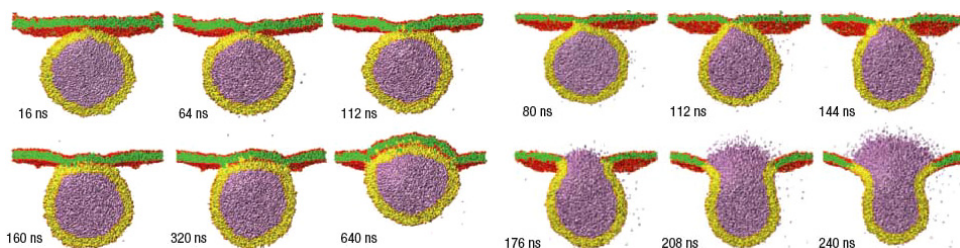


Fig. 5. Left: Adhesion of a tensionless vesicle and membrane. Right: Fusion event between a vesicle and a membrane. Reprinted by permission from Macmillan Publishers Ltd: Shillcock and Lipowsky [2005], copyright (2005).

fascinating DPD simulations for the fusion of vesicles to planar membrane patches, see Fig. 5. In Shillcock and Lipowsky [2005], they constructed a global morphology diagram, and more recently in Shillcock and Lipowsky [2007], they took into account the interactions between rigid nanoparticles and soft surfaces in their DPD modelling of membranes. The effect of chain length and asymmetry on the material properties of bilayer membranes was explored by Illya *et al.* [2005]. Later the dependence of the area stretch modulus and corresponding bending rigidity of binary mixture bilayers on their composition for various amphiphile packing parameters and tail lengths was also studied by Illya *et al.* [2006], and they found that the high curvature of the vesicles influences the evolution of the domain shapes. In Hong *et al.* [2007], the budding dynamics of individual domains in multicomponent membranes was studied using DPD simulations of varied bead number, and in Smith and Uspal [2007], the influences of shear flow on multicomponent vesicle was investigated.

Apart from the simulation of lipid bilayer membranes, DPD coarse grained modelling has also been used for the modelling of Nafion, [Yamamoto and Hyodo, 2003; Hyodo, 2004; Galperin and Khokhlov, 2006]. It has revealed a sponge-like bicontinuous structure of Nafion similar to the cluster-network model with the shape of the water regions not spherical but irregular, forming indistinguishable structures of water clusters and their channels. In LBM simulations of flow in Nafion polymer membranes, Hayashi *et al.* [2003] constructed the Nafion geometry data from results obtained prior by DPD simulations. Venturoli *et al.* [2005] developed an interesting DPD coarse-grained model for lipid bilayers with embedded peptides, and their model was used to study lipid-protein interactions as a function of hydrophobic mismatch. The review by Sperotto *et al.* [2006] can be referred to for a more detailed description of recent mesoscopic advances in simulation of lipid membranes with embedded or attached proteins.

2.4. Grafted polymer brush

Polymers grafted or absorbed on surfaces have many important technological applications including colloidal stabilization, lubrication, adhesion, wetting process and biocompatibility. These find applications in several industries such as automotive, lubrication and oil recovery where there are requirements to modify surfaces, friction and contact formation. Under good solvent conditions and high surface coverage, the attached polymer chains stretched strongly to the direction perpendicular to the grafted surface and polymer brushes are formed Goujon *et al.* [2004]. The structure and properties of these grafted polymer brushes were compared using MD and DPD by Pal and Seidel [2006], where results showed good agreement between the two methods, thus validating the applicability of the DPD technique to model relatively large length scale simulations of polymer brushes.

Malfreyt and Tildesley [2000] first used DPD to simulate grafted polymer brushes attached to a pore geometry of two walls of tethered DPD particles. Under equilibrium conditions in a good solvent, parabolic density profiles consistent with the self-consistent field (SCF) theoretical model were obtained. They also noted that as the solvent molecules were trapped in the entangled polymer, the diffusion along the pore axis was significantly higher for the solvent particles at mid-slab than those in the polymer/wall region. In addition, the effects of surface coverage on the overlap of the brushes, widths of the polymer brushes, stretch of chains and the ordering with respect to the surface normal were investigated. Similarly, Goujon *et al.* [2004] demonstrated that the DPD model in the grand canonical ensemble could be employed to simulate grafted polymer brushes under compression, and they calculated the force-distance profiles, which were found to be in very good agreement with SCF, as well as with experimental results of polystyrene brush layers grafted onto mica surfaces in toluene.

Wijmans and Smit [2002] studied the response of a brush to oscillatory shear flow, while Irfachsyad *et al.* [2002] investigated the effects of shear on grafted

polymers, in their DPD simulations. It was observed that with even the smallest shear rates, polymer chains preferred to align along the direction of the shear and to incline away from the surface normal. In an athermal solvent, the width of the grafted polymer chains decreased with increasing shear rate, whereas the layer shrank and there was no further decrease in width on shearing when in poor solvent conditions. Eventually it was found that reducing the quality of the solvent effectively reduced the width of grafted layers and the friction between them. Correspondingly through DPD simulations, Goujon *et al.* [2005] studied the effects of polymer grafting density, shear rate, nature of the solvent, steepness of conservative potential between polymer segments and the size of solvent particles on the force-distance and friction profiles.

Polymer coated channels can regulate solvent permeability by conformational changes of polymer brushes in response to stimuli. Consequently, Huang *et al.* [2006] studied solvent flow through these smart channels, see Fig. 6, and they were able to achieve a nearly 100-fold reduction in permeation through a proper choice of grafting parameters such as density and chain length. In addition, they investigated the height of the brushes in different solvent conditions under different pressure drops and found that under good solvent condition and low grafting density, the brush height decreases with the increase of the shear rate. Later the DPD simulations were performed by Qiao and He [2007] to study the effects of neutral grafted polymers on the modulation of electroosmotic flow. The simulated results could prove very useful to future design of polymer coating for flow control in micro/nano fluidic devices.

In Pastorino *et al.* [2006], molecular dynamics simulation of a short-chain polymer melt between two brush-covered surfaces under shear was carried out using the DPD thermostat. Consequently, the equilibrium density profiles, the behaviour under shear, the interdigitation of the melt into brush, the orientation on different length scales of free and grafted chains, and velocity profiles were investigated. Subsequently, via DPD simulations, Wu *et al.* [2007] studied the surface structures of conjugated rod-coil block copolymer brushes, and noted that the solvent quality, grafting density and rod-coil block ratio could control the photophysical properties of the brushes. In order to compare and characterize the behaviour of Langevin

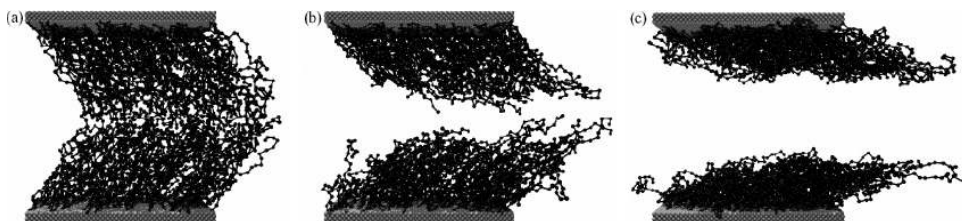


Fig. 6. Snapshots of polymer brushes, for different solvent quality, under solvent channel flow. Reprinted with permission from Huang *et al.* [2006]. Copyright 2006 American Chemical Society.

and DPD thermostats, Pastorino *et al.* [2007] conducted a series of simulations on model systems such as polymer brushes.

The properties of two opposing end-grafted charged polymer brushes in aqueous media under normal compression and lateral shear were studied by Sirchabesan and Giasson [2007]. Performing DPD simulations, they studied effect of the polymer molecular weight, degree of ionization, grafting density, ionic strength, and compression on the polymer conformation and the resulting shear force between the opposing polymer layers. It was observed that the friction coefficient was correlated to the extent of the interpenetration layer between the opposing polymer brushes directly. Moreover, it was found that the presence of electrostatic interactions and added counterions within the interpenetrated chains did not affect the friction force between sheared polymer beads.

3. Surfactant and Amphiphile Systems

Surfactants are of importance in many applications especially, when they absorbed onto the oil and water interfaces often to reduce the interfacial tension and promote mixing. It has been observed in the DPD simulations of Li *et al.* [2005a, 2005c] on surfactant monolayers at the interface between oil and water that for decreasing the interfacial tension, it would be better to have the same structure for the hydrophobic chains of surfactants and the oil since the molecule at the interfacial layer could array compactly.

Rekvisg *et al.* [2003a, 2003b] examined the effects of size and structure of surfactants on reduction of interfacial tension and in particular the influence of branching of the hydrophobic tail. In Rekvisg *et al.* [2003b], it was found that branching has a positive effect on the efficiency at the interface only if the head groups are sufficiently hydrophilic to prevent molecules staggering. Combining DPD with a Monte Carlo method, Rekvisg *et al.* [2003b] also determined the bulk concentrations in equilibrium with the interface, and from this they found that in order to reduce the interfacial tension by a given amount, it is necessary to increase the bulk concentrations of the branched isomers. Later, amphiphilic monolayers on the interface between oil and water was simulated by Rekvisg *et al.* [2004c] and their DPD simulations confirmed that the thickness of the layer affects the rigidity more than the density of the layer. They also found that mixtures of short and long surfactants are more flexible than medium length surfactants of the same average chain length. In Rekvisg *et al.* [2004a], the relation between the surfactant length n and the bending modulus of the monolayers κ was observed to obey the power law $\kappa \propto n^p$ with $p \approx 1.5$ at a constant surface density and $p \approx 1$ at a constant interfacial tension, which are consistent with mean field theory and available experimental data. Finally, for systems comprising two emulsion droplets separated by a film, [Rekvisg *et al.*, 2004b; Rekvisg and Frenkel, 2007] studied the surface forces, film rupture and droplet coalescence through DPD simulation of the interaction of oil/water/surfactant interfaces.

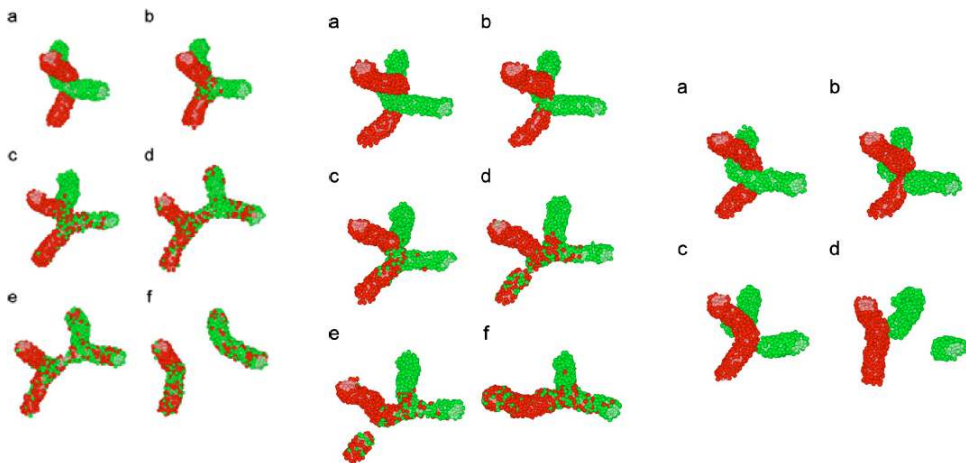


Fig. 7. Snapshots of time evolution of surfactant threadlike micelles. Left: phantom crossing process. Middle: micelle cut down at the branch point. Right: micelle break down at an entanglement point before the fusion process. Reprinted with permission from Yamamoto and Hyodo [2005]. Copyright 2005, American Institute of Physics.

Yamamoto and Hyodo [2005] investigated the crossing dynamics and possibility of a phantom crossing at an entanglement point of surfactant threadlike micelles in an aqueous solution, and it was confirmed through their DPD simulations that a moderate repulsive force between hydrophilic head groups could stabilize the threadlike micelle, see Fig. 7. More recently, the spontaneous formation process of threadlike micelles from the random configuration of surfactant molecules was studied Arai *et al.* [2007] and they observed that spherical micelles which were formed at early stages fused to each other and created threadlike micelles during the later stages. In Goicochea *et al.* [2007], the dependence of excess pressure and surface tension was studied for monomeric binary mixtures with the presence of surfactant at the interface. Also, the effects of surfactants concentration, salinity, and ratio of the two surfactants on the interfacial tension of the oil/water interface were considered by Li *et al.* [2007] through experimental analysis as well as DPD simulations.

3.1. Self-assembling systems of surfactants and amphiphiles

An area which has attracted numerous researchers to employ the mesoscopic DPD method widely over the last decade is the simulation of the self-assembly and aggregation of surfactants in solutions and the resulting equilibrium or non-equilibrium phases. Jury *et al.* [1999] were the first to employ DPD to simulate a dense solution of an amphiphilic species consisting of rigid AB surfactants in a solution of C monomers. They found a micellar phase, a hexagonal phase, a lamellar phase and a disordered structure which are very similar to phase kinetics of block copolymer

systems and their phase diagram was in line with experimental data. Similarly Nakamura [2004] obtained the phase diagram Jury *et al.* [1999] from his DPD simulation of amphiphilic molecules, and he also noted that the formation of the hexagonal phase takes longer time than the lamellar phase. Later, also by DPD simulations, Nakamura and Tamura [2005, 2006] investigated the hydrophilicity dependence of the phase structure more qualitatively by varying the interaction potential between hydrophilic molecules and water molecules.

In the mesophase formation from surfactant-water systems, Warren *et al.* [2003] found that the process is diffusion controlled. Subsequently, Guo and Kremer [2003] employed large scale parallelized DPD to simulate the phase behaviour of lamellar systems of diblock copolymers, surfactants and liquid crystals. Specifically, they used simplified amphiphile models such as *AB* dimers, *A2B2* tetramers and *A4B4* octamers. The application of DPD to simulate self-assembly of amphiphilic polymers and surfactants and formation of several kinds of microemulsions were later reported by Schulz *et al.* [2004]. Employing a coarse grained DPD model, Dong *et al.* [2004] studied the orientation of sodium dodecylsulfonate (DDS) and sodium dodecylsulfate (SDS), and they found that strong hydrophilic head groups and the addition of salt results in the surfactants being stretched and ordered. In Wang *et al.* [2005] mesostructures and morphologies of mixed surfactant solutions containing cationic gemini and anionic SDS was investigated and a variety of mesostructures, which were consistent with experiments, was reproduced by regulating the conservative term in the DPD algorithm Wang *et al.* [2005].

Dividing the *STS* and $C_{14}E_3$ surfactants into hydrophilic and hydrophobic DPD particles, the ionic and non-ionic mixed aqueous micellar systems were investigated by Kuo *et al.* [2004]. Wu *et al.* [2006] studied the self-assembly and morphology of the surfactant oligomers in an aqueous medium, and they observed that increasing the surfactant concentration will induce micelles transition from spherical and cylindrical phases and subsequently towards the lamellar morphological structure. Similarly, the DPD simulation results of Sun *et al.* [2006] on the aggregation of fluorinated surfactants showed that these surfactants have similar sequences of phases and aggregate micelle structures to that of their hydrocarbon analogues. During mesoscopic investigation of water morphology in reverse micelles, Yuan *et al.* [2004] arrived at the conclusion that DPD can be considered as adjuncts to experiments and provide microscopic information for the experiment. Performing both experiments and DPD simulations for the formation of vesicles from aggregated system of surfactants, Shang *et al.* [2006] found that almost all vesicles structures are multilamellar.

From the DPD simulations of Yang *et al.* [2006], different phase structures of an anionic surfactant aerosol *OT* mixed in water system were observed, and the influences of concentration and temperature on the phase behaviours of lamellar regions were studied. More recently, Huang *et al.* [2007a, 2007b] examined the phase behaviour of amphiphilic molecules in the presence of one or two

solvents. Their DPD simulations successfully predicted the overall phase transition behaviours under different composition of amphiphilic molecules and solvent selectivity/amount. However, it was also observed that the finite size of the simulation box could significantly affect the packing order of the spherical micelles such that it becomes a challenge for DPD simulations to examine the most stable packing array of spheres, as has been predicted by self-consistent mean-field theory.

3.2. *Polymers and surfactants in solution*

Due to various industrial applications like colloid stabilization or destabilization, flocculation and biotechnology, the interaction between ionic surfactants and water soluble polymers and their aggregation structures has attracted the attention of many researchers. Most of the phenomena that occur in these systems are in the mesoscale regime, making the DPD method an excellent technique for handling these systems. Using DPD, Groot [2000] comprehensively investigated the formation of polymer-surfactant aggregation in bulk solution and he observed two distinct modes of surfactant adsorption on the polymer. Molecular bottlebrush or swollen cage conformations were found when hydrophobic interactions are dominant while micellar structures on polymer formed when the binding between polymer and surfactant is dominated by surfactant headgroups. In addition, he represented the schematic phase diagram for the occurrence of various adsorption modes and found that as the surfactant concentration was increased, the polymer end point separation passes through a minimum. More complex systems such as those containing gold atoms as nanoparticle stabilizers were later considered by Juan *et al.* [2005] and Chen *et al.* [2007a, 2007b], also using DPD.

To explore the properties of polymer and surfactant system Yuan *et al.* [2003] selected two cationic surfactants and a polymer in their DPD simulations, and subsequently in Yuan *et al.* [2005], similar DPD simulations were applied for the investigation of other surfactant-polymer mixtures. The effects of pH value on the interaction between C14BE and Na-CMC in aqueous solution were studied by Li *et al.* [2005b] and they observed that aggregation is impossible at neutral pH = 7, while at pH = 2 due to stronger interactions the C14BE/Na-CMC aggregate is formed. More recently, Chen *et al.* [2007c] examined the behaviour and microstructure of the quaternary microemulsion system composed of Cetyltrimethylammonium bromide (CTAB)/octane/1-butanol/water, by DPD.

The sustained release of various drugs is an important issue in the design drug delivery systems and solid lipid microparticles (SLM) are micro/nano-scale drug carrier systems that can be used as efficient bio-compatible mechanisms for controlling and sustaining drug release. Optimizing the drug microstructure is a way to obtain the desired properties of a drug carrier. Long *et al.* [2006] conducted DPD simulations to model the aggregating morphology of SLM with tristearin, glyceryl behenate and cetyl alcohol as the carrier materials, and spherical, columnar, and lamellar structures were observed during low, moderate, and high oil contents

respectively. In addition, the ibuprofen distribution in the carriers was studied at low oil contents. More recently, Guo *et al.* [2007] investigated the effect of composition on aggregate morphologies of the drug-loaded microspheres, similarly using the DPD method.

Electrostatic interactions constitute the main interaction source between polymer and surfactant, and it is necessary to take them into account to predict the phase behaviour of mixtures of cationic, anionic and nonionic surfactants, and their interaction with polyelectrolytes Groot [2003]. Consequently Groot [2003] incorporated electrostatic interactions in his DPD simulation of a cationic polyelectrolyte solution. In the presence of salt, a fractal dimensionality was observed, while the polymer wraps around one or more discrete surfactant micelles when salt is replaced by an anionic surfactant. Later, using the standard Ewald sum method to calculate the electrostatic interactions within the DPD framework, González-Melchor *et al.* [2006] investigated the electrostatic interactions in a bulk electrolyte and polyelectrolyte-surfactant solutions.

4. Concluding Remarks

In this review, we have presented the major DPD works in the modeling and simulation of soft matter and polymeric systems. The works documented in this review account for those published either in-print or online, up to the end of 2007. Undoubtedly, due to the immense potential that the DPD technique holds, many more significant works will surface subsequently and it will be no surprise if the number of works involving the DPD increases exponentially, as the DPD technique continually finds new application areas and even new fields, where it can be applied and exploited.

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