

CHAPTER I

INTRODUCTION

Graphene is receiving large scientific attention, due to its exceptional properties (Shin et al., 2011), and significantly lower production cost over other carbon allotropes, such as carbon nanotubes (Xu et al., 2008). Unfortunately, strong dispersive attraction triggers agglomeration, especially when graphene sheets dispersed in polar solvents, which hinders many practical applications. Many methods have been proposed to stabilize graphene sheets (Liu et al., 2008; Xu et al., 2008; Hamilton et al., 2009; Bonaccorso et al., 2010; Green and Hersam 2010; Han et al., 2010). One is the use of surfactants, whose merit is stabilizing graphene inducing minimum surface defects (Min et al., 2012). Graphene is a planar sheet of carbon atoms, unlike fullerenes or carbon nanotube that possess curvature. The curvature can weaken the interaction between carbon atoms and surfactant molecules (Zhang et al., 2010). Therefore, graphene is capable of adsorbing more surfactants, compared with other allotropes (Bao et al., 2010; Tummala et al., 2010)

Many experiments related to SDS-aided graphene stabilizations have been reported (Rao et al., 2009; Subrahmanyam et al., 2009; Lee et al., 2010; Smith et al., 2010). Experimentally, visualization of SDS aggregates on graphene surface is obtained using atomic force microscopy (AFM), which cannot identify individual surfactants. Computer simulations can provide insights regarding the morphology of surfactant aggregates, which can aid practical applications. The main objective of this work is to utilize coarse-grained simulation techniques to study SDS aggregates on different graphene nanosheets. Our work builds on several recent contributions. For example, the aggregation behavior of surfactants and their self-assembly on carbonaceous nanoparticles have been studied via both molecular dynamic (MD) (Shelley et al., 1990; Mackerell 1995; Schweighofer et al., 1997; Bruce et al., 2002; Tummala et al., 2010; Lee and Kim 2012) and dissipative particle dynamics simulations (DPD) (Groot 2000; Angelikopoulos and Bock 2008; Calvaresi et al., 2009; Angelikopoulos et al., 2010). DPD offers the capability of simulating larger system, over longer period of time (Groot and Warren 1997), although it loses details that are observable using atomistic MD. In addition to pristine GS, we also simulated

partially reduced graphene oxide nanosheets, because there is an evidence for water accumulation around carboxyl groups on the edges of oxidized GS (Shih et al., 2012). We hypothesized that the presence of hydrophilic edges on the graphene nanosheets will affect the SDS aggregates. Another objective of this work is to study the agglomeration process of the graphene sheets, of different sizes, in different amounts of surfactant. The agglomeration of graphene sheets has been investigated via MD (Konatham and Striolo 2008; Shih et al., 2010; Park and Aluru 2011). Nevertheless, there have not been any coarse-grained simulations of SDS-aided graphene sheets stabilization so far.

This work consists of two sections. In the first section, we report the DPD simulation of the SDS aggregation on stationary graphene sheets (GS), graphene nano-ribbons (GN), graphene oxide sheets (GOS) and graphene oxide nano-ribbons (GON). In the second section, we present the simulation of GS aggregation, with different GS sizes and amounts of surfactants, in water