Asymptotic Analysis of Coagulation–Fragmentation Equations for Carbon Nanotube Formations

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Finding a manageable approximation to the behaviour of the coagulation–fragmentation equations is challenging [1]. The approximation is presented by means of asymptotic analysis, in a case that is simple to be studied, but realistic enough to be a good candidate as a model for physical processes [2]. The equilibrium difference between Gibbs free energies of interaction of an SWNT with its surroundings, in the solid phase and in the cluster volume, or on cluster surface, shows that on going from C_{60} (droplet model) to SWNT (bundlet) the minimum is less marked (55% of droplet), which causes a lesser number of units in SWNT ($n_{min} \approx 2$) than in C_{60} clusters (≈8) [3]. The abscissa is also shorter in SWNT (≈9) than in C_{60} clusters (≈28) [4]. With the packing-efficiency correction, the C_{60}–SWNT shortening decreases (68% of droplet) keeping $n_{min} \approx 2$ and $n_{abs} \approx 9$ [5]. The cluster distribution function by size in a solution of SWNT in CS_2, for saturation concentration at solvent temperature T = 298.15K, shows that on going from C_{60} (droplet) to SWNT (bundlet), the maximum cluster size decreases from n = 8 to 2 and distribution is narrowed, in agreement with the lesser number of units in SWNT clusters. With packing-efficiency correction, the distribution is narrowed keeping n_{max} = 2. The temperature dependence of solubility S of SWNT shows that S decreases with temperature because of cluster formation. At $T \approx 260$K, the C_{60} crystal presents a FCC to SC phase transition. The reduction is less marked for SWNT in agreement with the lesser number of units in clusters. At T = 260K on going from C_{60} (droplet) to SWNT (bundlet) S drops to 1.6% of droplet. With packing-efficiency correction the shortening decreases (2.6% of droplet). Based on a simple kinetic model and starting from the initial state of pure monomers, it is shown that the process of micellization of rodlike aggregates at high critical micelle concentration occurs in three separated stages or eras: (1) many clusters of small size are produced, (2) aggregates are increasing steadily in size and (3) a simple mean-field Fokker–Planck equation until the equilibrium distribution.

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