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Significant Effects of Confinement and Catalysis in Formation of Tabular Structures from Peapod Structures HAIBIN SU, R. NIELSEN, ADRI VAN DUIN, WILLIAM GODDARD III, Caltech — A large number of experimental and theoretical studies have been reported on buckyballs-containing nanotubes (a.k.a. peapod) structures since the discovery of these materials. It was observed that self- assembled buckyballs with nearly uniform centre-to-centre distances and resemble a nanoscopic peapod. The endofullerenes coalesce into longer capsules by either the electron irradiation or thermal annealing. We applied the recently developed Reactive Force Field (ReaxFF) to study the growth dynamic process starting from C_{60}-buckyball/nanotube peapod structures. We found that the space confinement provided by the single wall nanotube encapsulating the buckyballs, is of critical importance on the coalescence reaction. Furthermore, we also simulated the effects of a Ni-particles on the coalescence process and found a significant reduction on the reaction initiation temperature in the presence of these catalysts. One related quantity is the energy barrier of forming a 4-member ring between adjacent buckyballs. We chose both corannulenes ($C_{20}H_{10}$) and C_{60} to compute this energy barrier from quantum mechanic and ReaxFF. The good agreement between these two methods encouraged us to investigate the effect of catalysis on this energy barrier. It turned out that this barrier is lowered by 40% with the aid of catalysis. The piece of research work can help the community to gain better understanding of the complicated growth process in fullerene systems.

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