2. Nucleation, Growth and Healing Processes of Single-Walled Carbon Nanotubes

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1. Maeda and Ohno developed the global reaction route mapping\(^1\) (GRRM) method for automatic search of reaction pathways of type \(A \rightarrow X (+ Y)\). Recently we developed the artificial force induced reaction\(^2\) (AFIR) method for those of type \(A + B \rightarrow X (+ Y)\). These methods can be used not only for exploring TS structures for a single PES but also for locating minima and saddle points on the seam of crossing (MSXs) including conical intersections. Some applications to organic multicomponent reactions, photodissociation reactions of aldehydes and ketones,\(^3\) and the roaming dynamics on excited electronic states\(^4\) will be also presented.

2. We review our quantum chemical molecular dynamics (QM/MD)-based studies of carbon nanostructure formation under nonequilibrium conditions.\(^5\) We find that carbon nanostructure formation from feedstock particles involves a phase transition of sp to sp\(^2\) carbon phases, which begins with the formation of Y-junctions, followed by a nucleus consisting of pentagons, hexagons, and heptagons. The dominance of hexagons in the synthesized products is explained via annealing processes that occur during the cooling of the grown carbon structure, accelerated by transition metal catalysts when present. The dimensional structures of the final synthesis products (0D spheres – fullerenes, 1D tubes – nanotubes, 2D sheets – graphenes) are induced by the shapes of the substrates/catalysts, and their interaction strength with carbon.