Nucleation of soot nanoparticles from polycyclic aromatic hydrocarbon precursors

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Understanding of the soot formation process is crucial for reduction of harmful emissions from combustion and also for synthesis of various important carbon structures. It is widely accepted that nucleation of carbon nanoparticles in flames comes via intermediate stage of formation of polycyclic aromatic hydrocarbons (PAHs) and their dimerization, but still precise physical and structural properties of the nanoparticles in the early stages of formation and nucleation mechanism still remain unknown. In this work we describe nucleation kinetics of soot particles formed from large PAH structures with more than 60 atoms. Molecular dynamics simulations with reactive potential ReaxFF [1] were performed in temperature range 2000–2700 K. Structure of soot nanoparticles is examined by comparing parameters such as hybridization, H/C ratio, distribution of carbon fringe length and tortuosity. In addition, we examine how formation temperature affects the particle morphology and thermal stability.

[1] Chenoweth K, Van Duin A C and Goddard W A 2008 *J. Phys. Chem. A* **112** 1040–1053