Kinetics of carbon soot growth from polycyclic aromatic hydrocarbon precursors: Atomistic modeling

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Soot formation have a great impact on such processes as fuel combustion and synthesis of carbon structures. Nevertheless, the formation and growth of soot structures have not been understanded well [1, 2]. The collisions between soot particles and different hydrocarbon molecules are valuable for understanding the process of soot particles growth. We examine how the morphology of soot nanoparticles formed at different temperatures (in the range $T = 2250$ to 3000 K) influence their ability to adsorb PAHs (polycyclic aromatic hydrocarbons) from the gas phase and how it affects the growth kinetics in general. This way, we study the energy of the interaction between PAH molecules and soot. The results were obtained using LAMMPS with ReaxFF [3] potential.

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[2] Mao Q, van Duin A C T and Luo K H 2017 *Carbon* **121** 380–388
[3] Van Duin A C T 2001 *J. Phys. Chem. A* **105** 9396–9409