Mechanisms of soot thermal decomposition: insights from reactive molecular dynamics

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Understanding the mechanisms of soot formation and decomposition is important for reduction of harmful emissions from combustion. Soot sublimation temperature varies in a wide range from approximately 2500 to 4500 K and the fundamental reasons for such drastic discrepancy are still unknown. In our paper [1] we model thermal decomposition of soot using reactive molecular dynamics simulations to shed light on the relationship between soot morphology and its sublimation temperature and to study the molecular products of its sublimation. Our results show that besides well-known low-molecular-weight C_1–C_5 species [2, 3] soot can also decompose into graphene-like products with mass up to 300–600 Da. Mass distribution of the sublimation products strongly depends on the morphology of the particle which in turn depends on the conditions at which the particle was formed. Moreover we demonstrate that those soot particles which can withstand temperatures up to 3000 K undergo fast annealing which additionally enhances their thermal stability.

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