An Image-Guided Rapid Soot Structure Construction Strategy

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Abstract
The relationship between soot reactivity and structure is difficult to explore via atomistic simulations due to the lack of construction tools to address spherical particles with multiple-shells, and a wide range of molecular sizes. Here we propose an image guided shell-by-shell construction approach. The structure is informed from image analysis of HRTEM lattice fringe micrographs with shell radii, d-spacing, PAH size distribution, and circumference coverage being established. A python script uses the desired radius, PAH distribution, and desired coverage area as inputs for a shell-by-shell construction approach. The molecules are randomly "placed" on the spherical surface (a calculation rather than actual placement), without overlapping. The molecules are "added" sequentially in descending order of size. Once the "placement" has been established, the spherical coordinates are converted into Cartesian space with Fringe3D providing the actual construction. This Perl script places the centroid of molecules in 3D space, adds the atoms, rotates, and pitches the molecule in the desired manner. The combination of these approaches provides a measure of control for the rapid construction of multiple shell soot structures. Here an example coal-derived soot structure (18 shells of radii between ~85 to 150Å) is constructed with flat PAH molecules (ignoring curvature, heteroatoms, and cross-links) raging in size from coronene to 864 carbon atoms (~350 rings). This simplistic structure can be constructed in a day or two following image analysis. This provides an elegant approach for further exploration of combustion/gasification reactivity.