Generation and characterization of an improved carbon fiber model by molecular dynamics

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A high-fidelity carbon fiber model is necessary for understanding the microstructure and investigating the mechanical properties of carbon fiber at the atomic scale. We present an approach for generating non-periodic carbon fiber microstructures (thin fiber) based on the periodic carbon fiber model (core fiber) developed by Desai et al[1], enabling further exploration of the interface properties between carbon fiber and other materials such as resin, amorphous carbon, and char. This improved carbon fiber model is capable of producing carbon fiber microstructure at wide range densities from 1.6g/cc to 2.0g/cc. A systematic characterization of the microstructure of core fiber and thin fiber is undertaken by evaluating the hybridization state of carbon atoms, the pore size distribution, population of carbon rings, graphitization degrees and bond angles. The virtual X-ray diffraction pattern is computed and is in good agreement with the available experiment data for carbon fiber. Further, we develop a strength reduced carbon fiber model by artificially introducing defects in the axial direction to decrease the extreme high tensile modulus. Finally, we predict the tensile moduli of the strength reduced carbon fiber model between 200-400Gpa matching those of PAN-based carbon fibers. We find that the periodic core fiber have a higher tensile modulus compared with nonperiodic thin fiber model at the same density proving that failed thin fiber surface reduce the tensile modulus.

Keywords: Carbon fiber, Molecular Dynamics, Characterization

[1] Desai, S., Li, C., Shen, T., & Strachan, A. (2017). Molecular modeling of the microstructure evolution during carbon fiber processing. The Journal of chemical physics, 147(22), 224705.