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New Algorithms for Particle-in-Cell Simulations of Carbon Nanotubes Growth in Flowing Plasma.[1] SERGEY AVERKIN, Tech-X Corp — Plasma, such as arc discharge plasma, is known as an effective environment for the production of carbon nanotubes (CNTs) and other nanomaterials. It is believed that the plasma-induced production enhancement, relative to conventional chemical vapor deposition reactors, is due to the presence of free radicals and ions that can contribute (along with neutral atoms and molecules) to nanoparticle growth. Numerical simulations of plasma around nanoparticles at kinetic scales can shed light on the underlying physical mechanisms that contribute to nanoparticle growth, thus enabling better prediction and control of nanomaterial production. In this work we present numerical algorithms for simulation of CNT growth in flowing plasmas, as implemented in Tech-X Corporation's commercial particle-in-cell code VSim. We also exercise these algorithms in simulations which explore the effect of the plasma drift velocity on the nanoparticle growth. The new numerical algorithms include extended surface chemistry, efficient remeshing of the simulation domain, and a new formulation of flux boundary conditions based on the Kinetic-Moment boundary condition framework originally developed for the Direct Simulation Monte Carlo (DSMC) method.

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Sergey Averkin
Tech-X Corp

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