Abstract Submitted
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Particle in Cell Simulation of Plasma Assisted Carbon Nanotubes Formation[1] SERGEY AVERKIN, Tech-X Corporation, University of Colorado Boulder — Nano materials have a wide range of applications, ranging from drug delivery in medical applications to new composite materials in aerospace applications. Experimental data on nanoparticle growth exists, but numerical simulations are needed to understand the underlying physical mechanisms and to enable better prediction of nanomaterial production. The numerical models of plasma assisted production span from detailed atomistic models including interaction of individual atoms to fluid models coupled with Maxwell equations that determine plasma composition and kinetic models describing the nanoparticle growth. However, existing models are either computationally extremely expensive as in the case of atomistic models or don't include kinetic effects that are important for the nanoparticles production. We present Particle-In-Cell (PIC) simulations of growth rates of carbon nanotubes using commercial software VSim. Because PIC is less computationally expensive than atomistic simulations and can still capture kinetic effects that fluid simulations cannot, it is able to address this important issue in a unique way. In addition, PIC predictions can be fed to existing plasma fluid codes for more accurate production modeling.

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