Abstract Submitted
for the GEC19 Meeting of
The American Physical Society

Progress in Particle-in-Cell Simulations of Plasma-Assisted Carbon Nanotubes Formation[1] SERGEY AVERKIN, Tech-X Corporation — Nanomaterials such as carbon nanotubes (CNTs) have a wide range of applications ranging from water purification to new composite materials. The use of plasmas for nanomaterial generation has many advantages compared to conventional chemical vapor deposition, such as the presence of reactive species that allows lower operational temperature during production. While there is extensive experimental data on nanoparticle growth in plasmas, in many cases fundamental understanding of the underlying physical processes is lacking. Numerical simulations can shed light on the underlying physical mechanisms and enable better prediction of nanomaterial production. We present progress in the Particle-in-Cell (PIC) simulation of CNTs growth in a plasma environment. We use the commercial PIC code VSim, with extended surface chemistry, in order to simulate growth of a single CNT in the plasma environment. We use remeshing of the simulation domain to track changes in the CNT surface due to its growth; this allows us to capture changes in the particle fluxes. The augmented surface boundary conditions include surface diffusion, adsorption and desorption. VSim predictions of the CNT growth rates can be fed to existing plasma fluid codes such as USim for more accurate production modeling.

[1]Sponsored by US DoE SBIR Award DE-SC0017842

Sergey Averkin
Tech-X Corporation

Date submitted: 03 Jun 2019 Electronic form version 1.4