# Aerospace Engineering Dissertation Defense

## Investigation of Plasma Source for Nanoparticle Synthesis

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# Abstract

Silicon nanoparticles (SiNPs) have emerged as promising next-generation anode material for lithium-ion (Li-ion) batteries owing to their exceptionally high theoretical capacity of 4200 mAh/g. However, large scale and cost-effective manufacturing of SiNPs with controlled size and morphology requires a fundamental understanding of the plasma processes governing their formation. Plasma assisted synthesis offers distinct advantages in producing high-purity uniform nanoparticles. The underlying physics of high-pressure radiofrequency (RF) driven discharges used in such systems remain insufficiently characterized.

This research presents the development and validation of a continuum, two-dimensional, axisymmetric computational model to simulate the plasma source used in RF assisted SiNPs synthesis. The model builds upon NASA-Jet Propulsion Laboratory's (JPL) Orificed Cathode Two-Dimensional (OrCa2D) code originally designed for xenon direct current (DC) hollow cathode discharges and extends its capabilities to argon RF plasmas. Major upgrades include the incorporation of argon specific collisional cross-sections, Faraday induced azimuthal electric field formulation, electromagnetic coupling with an RF circuit, and the addition of boundary conditions suited for floating plasma walls. The upgraded solver was implemented with a magnetic field aligned mesh (MFAM) to capture transport in a collisional, partially magnetized plasma operating near 4-5 Torr and 13.56 MHz.

Model predictions were validated against experimental measurements obtained using an RF-compensated double Langmuir probe in an argon plasma source operating at 5.5 Torr and 100 W. The measured number density values (~10^10-10^11 cm^(-3)) and temperatures (~1.25 eV) compared very well to the simulated plasma two-dimensional, steady state distributions. Grid-convergence and temporal stability studies confirmed the robustness of the upgraded numerical framework.

The validated computational tool was applied to investigate the effects of varying operating pressure, power level and frequency. It concluded that pressure variations weakly affect plasma production, while frequency and power level settings at 100W and 13.56MHz approximately represent optimum operation. The present state of the code represents the foundation for the development of an adequately predictive capability that will mature upon inclusion of mixture chemistry and clustering mechanisms.

November 7, 2025; 11:30am; DH L1-09

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