DOE Plasma Science Center

Visiting Graduate Student/Post Doctoral Researcher Fellowship Report

Title of Project:	Numerical simulation of 2D capacitively-coupled RF plasma for the synthesis of silicon nanocrystals	
Name:	Romain Le Picard	
Institution:	University of Minnesota	
Email:	rlepicar@umn.edu	
Advisor:	Steven L. Girshick	
Advisor email:	slg@umn.edu	
Institution Visited:	University of Michigan	
Host:	Mark J. Kushner	
Host email:	mjkush@umich.edu	
Dates of Visit:	**Start: 03/30/2015**	**End: 04/03/2015**

I. Description and Importance of Research Issues Investigated During Visit

I visited Kushner's group from March 30th to April 3rd, 2015, to work on numerical simulation of 2D capacitively-coupled RF plasma for the synthesis of silicon nanocrystals (SNCs). This work is based on the collaboration of Girshick's group (University of Minnesota) and Kushner's group (University of Michigan).

SNCs can be produced in capacitively coupled RF plasmas. Many experimental studies have been done to understand formation and growth of SNCs within a plasma. However, only recently have self-consistent numerical simulations of SNC formation in a plasma been reported. Our objective is to model SNC formation and growth in a 2D self-consistent plasma of the type reported in Ref. [1].

This visit to Michigan was focused on several aspects of the integration of the Plasma Aerosol Model of Girshick's group with the Hybrid Plasma Equipment Model of Kushner's group:

1. Change boundary conditions at the outlet to avoid the trapping of negative ions in the plasma
2. Modify the INEUTRAL_NOPLASMA option to gain a speed-up by updating all heavy species densities, while keeping plasma parameters constant

The work has been done with Dr. Aram Markosyan.

II. Discussion of Research Outcomes and Findings Resulting from Visit

During the visit, the following has been accomplished:

- **Boundary condition at the outlet**

In the previous version, the outlet material was metal and grounded. It induced a drop in potential which trapped negative species. As a result:

1. Nanoparticle could not leave the plasma region
2. Nanoparticle size was overestimated

We modified the geometry to impose the axial gradient in potential at the outlet to be zero. Potential are shown in figure 1. Streamlines for the negative nanoparticle (D=0.5nm) are shown on figure 2.

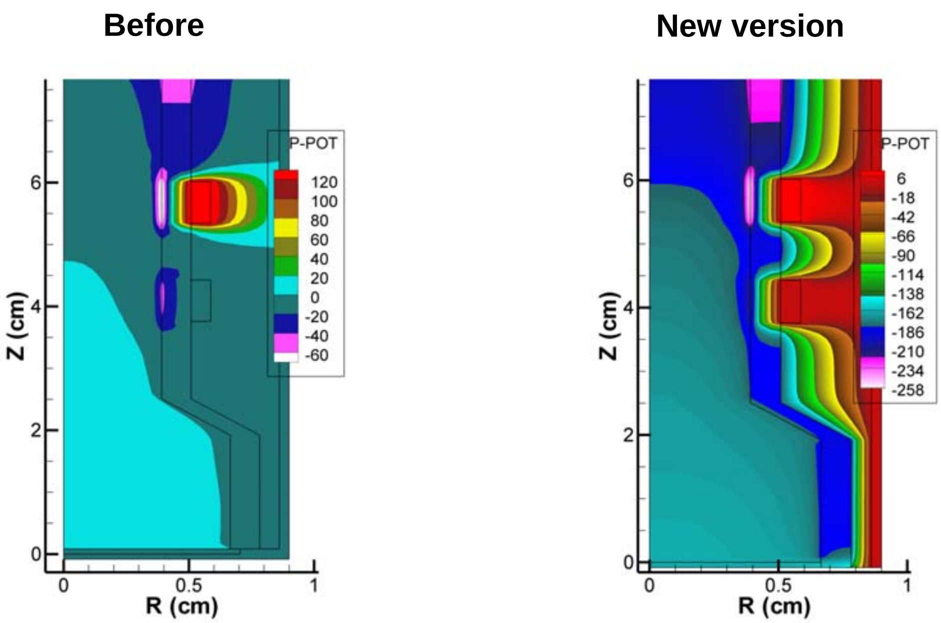

Figure 1 Comparison of the potential near the outlet between previous version (left) and the new version (right)

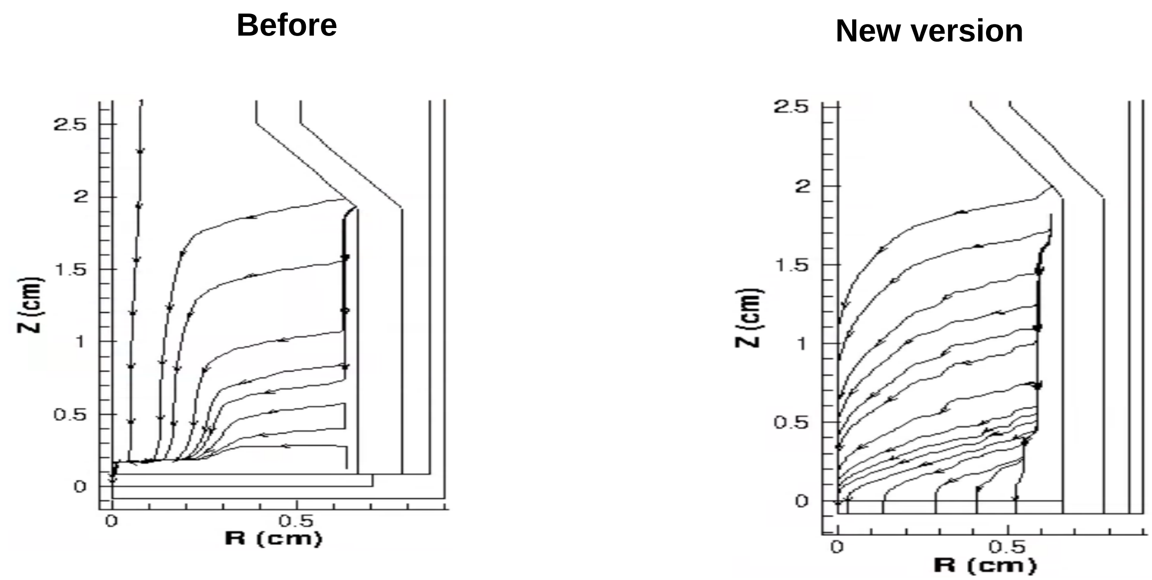

Figure 2 Streamlines for a 0.5 nm-diameter particle for the previous version (left) and the new version (right)

- **INEUTRAL_NOPLASMA option**

The option INEUTRAL_NOPLASMA is used at the end of each iteration to solve the population balance equation of neutral species only, while keeping plasma parameters constant. It can decrease the convergence time.

In the experimental plasma conditions, nanoparticles are mostly negatively charged. Therefore, we extended this option for neutral and charged species, except electrons.

III. Followup to visit

- **Boundary condition at the outlet**
    1. Run a long case with one section and see if nanoparticles remain trapped at the outlet
    2. Run longer cases for 30 and 50 sections

- **INEUTRAL_NOPLASMA option**
    1. Make the code work with the option for only neutral species
    2. Make the code work with the option for neutral and charged species

We will also parallelize aerosol subroutines.

References

[1] L. Mangolini, E. Thimsen, U. Kortshagen, *Nano Lett.,* vol. 5, 655- 659, 2005.
[2] P. Agarwal and S. L. Girshick, *Plasma Sources Sci. Technol.,* vol. 21, 055023, 2012.