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	
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Host:	Mark J. Kushner	
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Dates of Visit:	**Start: 11/13/2013**	**End: 11/15/2013**

I. Description and Importance of Research Issues Investigated During Visit

We visited Kushner's group from May 13th to 15th, 2013, 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 and Kortshagen's groups (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]. SNCs grow by coagulation and surface growth. 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.

II. Discussion of Research Outcomes and Findings Resulting from Visit

During the stay, the restructuring of the code and the implementation of external forces were accomplished.

- **Code restructuring**

To ease the collaboration between Kushner's and Girshick's groups, as well as the maintenance of HPEM, the code has been restructured. All subroutines have been implemented in the same file hpem_aero.f.

- **Implementation of external forces**

Inclusion of two external forces was implemented during the stay.

The ion drag force results from the momentum transfer from ions to aerosol particles, by (1) collection and (2) orbital force. The expression for the collection force is:

$$F_c = \pi a^2 n_i m_i v_T v_i \left[1 - \frac{2eV(a)}{m_i v_T^2}\right],$$

where a is the aerosol radius, n_i the ion density, m_i the ion mass, v_t the total velocity, v_i the ion drift velocity, and $V(a)$ the dust particle potential.

The expression for the orbital force is:

$$F_o = n_i m_i \sigma_0 v_T v_i,$$

where σ_0 is the momentum transfer cross section.

The neutral drag force is due to momentum transfer from gas molecules with dust particles. This is defined as:

$$F_N = -\frac{4}{3}\pi a^2 m_g n_g v_g (u_D - u_g)\left(1 + \alpha\frac{\pi}{8}\right),$$

where α is an accommodation factor.

III. Followup to visit

Integration of all modules has now been implemented: nucleation, coagulation, surface growth, and external forces (ion and neutral drag). After verifying whether these modules perform correctly, a number of simulations will be run for different numerical parameters (number of aerosol sections, coefficients…) and plasma parameters (power, boundary conditions…). The code will be sped-up by parallelizing the aerosol modules.

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.