*DOE Plasma Science Center*

**Visiting Graduate Student/Post Doctoral Researcher Fellowship Report**

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| **Title of Project:** | Numerical simulation of 2D capacitively-coupled RF plasma for the synthesis of silicon nanocrystals | |
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| **Dates of Visit:** | **Start: 05/28/2013** | **End: 05/31/2013** |

## I. Description and Importance of Research Issues Investigated During Visit

I visited Kushner's group from May 28th to 31st, 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 works have been done to understand formation and growth of SNCs within the plasma. However, the literature does not report any involved numerical simulations of SNCs formation and growth in self-consistent plasma. Our objective is to model SNCs formation and growth in 2D self-consistent plasma from Ref. [1]. SNCs grow by coagulation and surface growth. This is possible because of large residence time, due to their negative charge. Indeed, the electric field can confine them inside plasma for a "long" time. The main purpose of this visit to Michigan was included the dust charging model.

## II. Discussion of Research Outcomes and Findings Resulting from Visit

During the stay, general notation convention has been discussed first. Following, we discussed charging model and anticipated both coagulation and surface growth models.

- **Notation convention**

Dust particle formation and growth uses sectional model with different particle charge distributions in each section [2]. The name of a particle of given size and charge has the form AEXXYYZ, where AE stands for AErosol particle, XX for section, YY for charge number, and Z for negative(-) or positive(^). For example, AE0100 is section "1" and charge number "0" (i.e. neutral). AE0101- is section "1", charge number "1" negative "-". AE0101^ is section "1", charge number "1", and positive "^". AE1306- is section "13", charge number "6", and negative "-".

Reactions are identified by special numbers. For convention we decided: 100000 for ion charging rates, 7001-7499 for electron elastic collisions, 7501-7999 for electron attachment to particles. Every single reaction involving electrons needs a different special number.

- **Electron-dust cross section**

Electron cross sections where find in [3]. Electron-dust elastic cross section is defined as:

$$\sigma_{ed}^{\varepsilon}(\varepsilon) = \pi R^2(-\phi_s/\varepsilon)^2 e^{2R/\lambda_D} \ln\Lambda,$$

where $R$ is the radius, $\phi_s$ the surface potential, $\varepsilon$ the energy, $\lambda_D$ the Debye length, and $\Lambda \approx -\lambda_D T_e / R\phi_s$.
It depends on plasmas parameters (e.g. electron density, electron temperature). However, in the current version of HPEM, cross sections are not calculated at each cell of the plasma. An average Debye length is therefore calculated, and we will use it. Modifications will be done to the code later on.
Electron attachment to particle is expressed as:

$$\sigma_{ed}^{c}(\varepsilon) = \pi R^2 (1 + \phi_s/\varepsilon),$$

for $\varepsilon \geq -\phi_s$ and 0 otherwise.
To strengthen our model, electron energy distribution function will now be solved via a Bolztmann solver in HPEM. Monte-Carlo solver will be a possible alternative in future. However, this option may be too computationally intensive. Electron current to particle is therefore defined as

$$I_e = \pi R^2 e n_e \int_{-\phi_s}^{\infty} \left(1 + \frac{\phi_s}{\varepsilon}\right) \sqrt{\frac{2e\varepsilon}{m_e}} F_0(\varepsilon) \sqrt{\varepsilon} d\varepsilon,$$

where $F_0(\varepsilon)$ is the electron energy distribution function.

- **Ion current to particles**

In our model, particle charging is done by solving particle charge balance equation. Ion current particle is found by the Orbit Limited Theory (OML), in which ion energy distribution function is supposed to Maxwellian [4]. In our current 1D model, electron energy was also assumed Maxwellian [2]. We consider singly positively charge dust particles.
Within this model, electron and ion currents depend on the number of charge $z$ carry by nanoparticles and are fully described by electron and ion densities ($n_e$, $n_i$), temperatures ($T_e$, $T_i$) and masses ($m_e$, $m_i$). Depending of surface potential, currents to particle for $V_s<0$:

$$I_i = I_{0i}(1 - eV_s/kT_e),$$

And for $V_s \geq 0$:

$$I_i = I_{0i} \exp(-eV_s/kT_e),$$

where $I_{0e}$ and $I_{0i}$ are electron and ion currents at $V_s=0$, and $I_{0x} = \pi R^2 n_x (8kT_x/\pi m_x)^{1/2}$ for $x \equiv e,i$.
The rate of ion attachment to particle is done in subroutine RATESUB. All reactions are in icp.dat. A special number 100000 is given for ion attachment to particles. An example of ion reaction is:

Ar^ + AE0100 > AE0101^ + AR3S,

where AR3S is argon ground state.

- **Coagulation and surface growth anticipation**

We will be able to extend method described in above bullet points for coagulation and surface growth models. The special number 100001 will be given for coagulation. The special number for surface growth is 100002.

**III. Follow-up to Visit**

Nucleation and charging models have been successfully included in the current version. Nucleation occurs with negative ions as $SiH_2^-$ and $SiH_3^-$. Therefore, we will need to account for it and get a better set of chemical reactions leading to nucleation. Coagulation and surface growth will be added thereafter.

**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.
[3] I. Denysenko, M. Y. Yu, K. Ostrikov, and A. Smolyakov, *Phys. Rev.,* vol. 70, 046403, 2004.
[4] J. E. Allen, *Phys. Scripta,* vol. 45, 497, 1992.