DOE Plasma Science Center

Visiting Graduate Student/Post-Doctoral Researcher Fellowship Report

Title of Project:	Modeling of vibrational kinetics in Cl_2 inductively-coupled plasmas	
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Institution Visited:	Mich. Inst. for Plasma Sci. & Engr. (MIPSE)	
Host:	Mark Kushner	
Host email:	mjkush@umich.edu	
Dates of Visit:	**Start:** October 6 2013	**End:** October 27 2013

I. Description and Importance of Research Issues Investigated During Visit

Chlorine-based plasmas are of great industrial importance for the etching of silicon in the fabrication of CMOS integrated circuits. An accurate model of this system is necessary to enable improved reactor design and process development.

Experimental results were obtained at LPP with an industrial scaled ICP reactor. The electron density radial profile was measured using microwave resonator hairpin probe, and the chlorine atom density was measured using Laser-Induced Fluorescence. The neutral gas temperature was also measured using laser diagnostics. The experimental results were compared to 2D Hybrid Plasma Equipment Model (HPEM, developed by Mark Kushner) simulations in November 2011 and significant disagreement was observed. These original simulations did not include the kinetics of vibrationnally excited states. The calculated gas temperature was too low and as a consequence the simulated electron density profiles are too localized, at least at pressures above 20 mtorr.

We have postulated that vibrational kinetics have a great impact on gas heating in the plasma. A model of the vibrational kinetics and its impact on gas heating was proposed and tested using global models.

The aim of the visit was to implement this vibrational kinetics model in HPEM and compare the new HPEM results with experimental data from LPP reactor and global model results.

II. Discussion of Research Outcomes and Findings Resulting from Visit

The vibrational kinetics in chlorine plasmas can be an important process on gas heating. The vibrational excitation is obtained through electronic collisions which pass by a transient anion $(Cl_2^-)^*$ and can produce a higher vibrational level or dissociative attachment.

The gas heating is produced with the transfer of vibrational energy to the translational energy through collisions with chlorine molecules or atoms (these transfers are more efficient with chlorine atoms).

The different studied models are:

- HPEM without any vibrational kinetics (HPEM nov 11),
- HPEM with simple vibrational kinetics (v=0, 1, 2 and no impact on attachment, HPEM mar 13),
- HPEM with complex vibrational kinetics (up to v=5, HPEM nov 13),
- A global model (without gas heating equations), with complex vibrational kinetics (up to v=5).

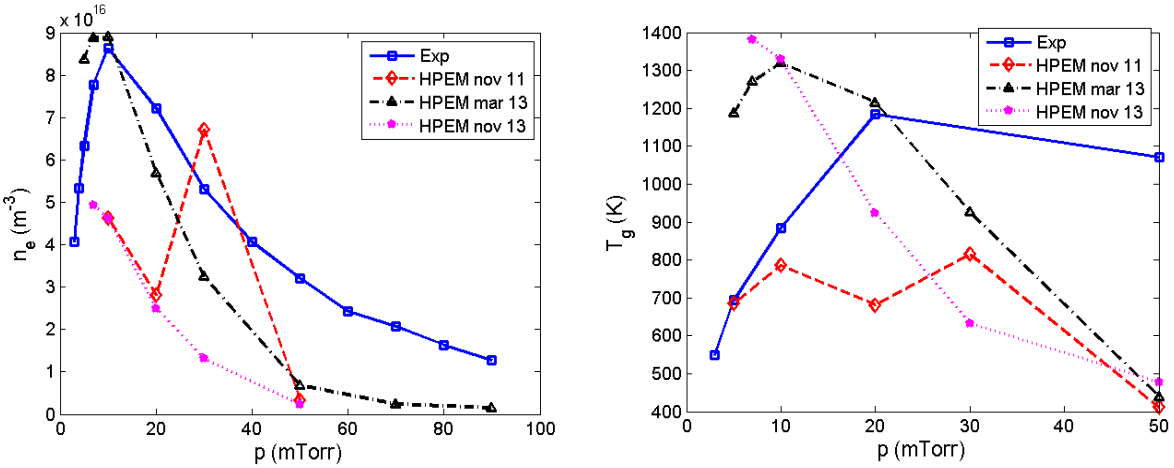

Figure 1. Electronic densities (left) and gas temperature (right) at P=500 W.

The figure 1 shows the evolution of the electron density and the gas temperature at the reactor center, for the various HPEM simulations and for experiments. As mentioned above, the neutral gas temperature was underestimated by the original HPEM simulations (Nov 2011, red curve), except at the lowest pressure. The lower gas temperature (and thus the higher neutral densities) resulted in lower electron density in the center due to the slowest diffusion of the plasma, as shown in figure 1, and in figure 2.

The implementation of a simplified vibrational kinetic scheme in HPEM, in March 13, led to higher neutral gas temperature and consequently to a higher electron density. The agremment with experiments was improved, although the neutral gas temperature is now too high at the lowest pressure. These simulations included the effect of vibrationally excited states on gas heating but not on the electron attachment, such that the negative ion density remained fairly unchanged.

During the visit, a more sophisticated vibrational kinetic scheme was incorporated leading to the HPEM nov 13 results also shown in figures 1&2. This led to lower gas temperatures at higher pressure again, bringing the simulations results closer to the original nov 2011 HPEM results. However, at the lowest pressure the simulations predict high gas temperature, without a

significant effect on the electron temperature. This somewhat surprising result is due to the higher negative ion (Cl^-) density predicted by the nov 2013 simulations. Indeed, attachment on vibrationnally excited states is high which leads to Cl- densities above 10^{17} m^{-3}.

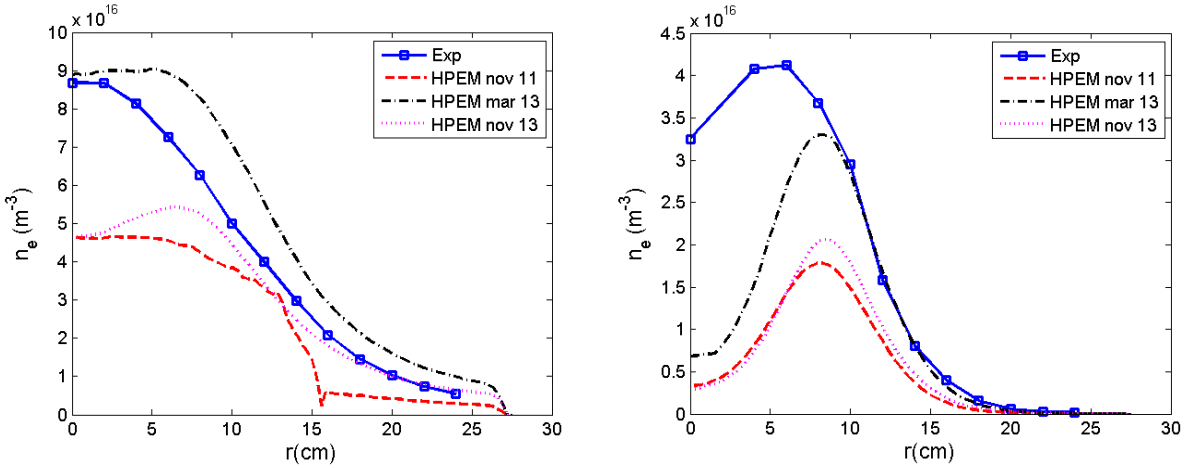

Figure 2. Radial distribution of electronic density at p=10 mTorr (left) and p=50 mTorr (right) for P=500 W.

The electron density, the Cl^- density and the vibrationnal temperature are shown in figure 3 for the nov 2013 HPEM simulations and for a global model having the same chemical reaction scheme. We observe a fairly good agreement for the electron density and a decent agreement for the vibrational temperature. The agreement is less good for the negative ion density; the trends with pressure are not captured, although the absolute values are close. This is not entirely surprising because the global model does not work well at high pressure in a large plasma chamber, for which spatial variations are very important.

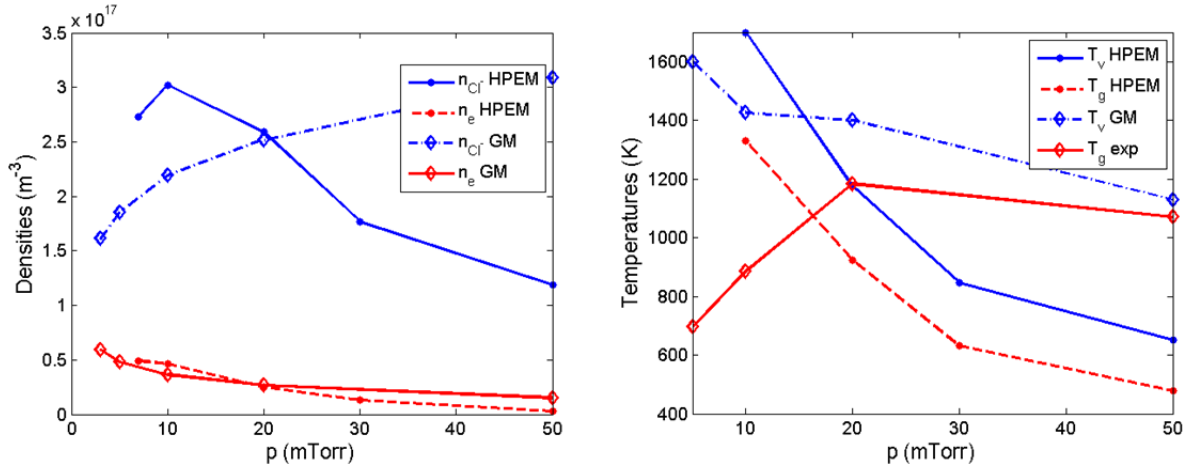

Figure 3. Cl^- density (left) and vibrational temperatures (right) as function of pressure at P=500 W.

III. Follow-up to Visit

As we can see in this short report, the first attempts to include a reasonable vibrational kinetic scheme in HPEM are still unsatisfactory. Additional work is required and the LPP team is still working on the subject, in close collaboration with Mark Kushner at University of Michigan. In particular, the role of capacitive coupling at low power should also be investigated because it could also play an important role in the discrepancy between experiments and simulations (capacitive coupling is not included in the simulations presented in this short report).

The visit was however very fruitfull because Benjamin and the LPP team have increased their understanding of HPEM and the whole team has improved his understanding of the vibrational kinetics in Cl_2 plasmas. The subject is of great interest and we expect a long-term collaboration between the two teams, with cross visits, eventually leading to publications in peer-reviewed journals.