PIC Simulations of α to γ Transition in Atmospheric Pressure Capacitive Discharges

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Atmospheric pressure capacitive micro-discharges are of interest due to emerging applications, especially in the bio-medical field. A previous global model did not consider high power phenomena such as sheath multiplication, thus limiting its applicability to the lower power range. To overcome this, we use 1D particle-in-cell (PIC) simulations of atmospheric He/0.1%N_2 capacitive discharges over a wide range of currents and frequencies to guide the development of a more general global models which are also valid at higher powers. The new model includes sheath multiplication and two classes of electrons: the higher temperature "hot" electrons associated with the sheaths, and the cooler

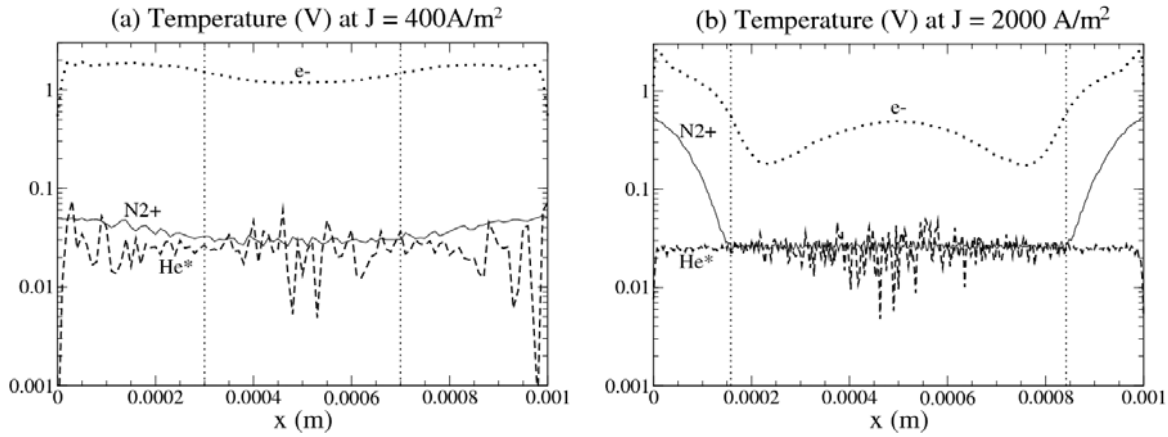

Fig. 1 – Time-averaged PIC results at 27.12 MHz, showing particle temperatures for a low power α mode case with (a) J= 400 A/m^2 and a high power γ mode case with (b) J=2000 A/m^2. The dotted vertical lines are at x = s_m and x = L - s_m, where L = 1mm is the discharge length, and s_m is the maximal sheath width for each case.

"warm"' electrons associated with the bulk. The electric field and the electron power balance are solved analytically to determine the time-varying hot and warm temperatures and the effective rate coefficients. The particle balance equations are integrated numerically to determine the species densities. The model and PIC results are compared, showing reasonable agreement over the range of currents and frequencies studied. They indicate a transition from an α mode at low power characterized by relatively high electron temperature T_e with a near uniform profile to a γ mode at high power with a T_e profiles strongly depressed in the bulk plasma. (See Fig. 1.) The transition is accompanied by an increase in density and a decrease in sheath widths. The current and frequency scalings of the model are confirmed by the PIC simulations.

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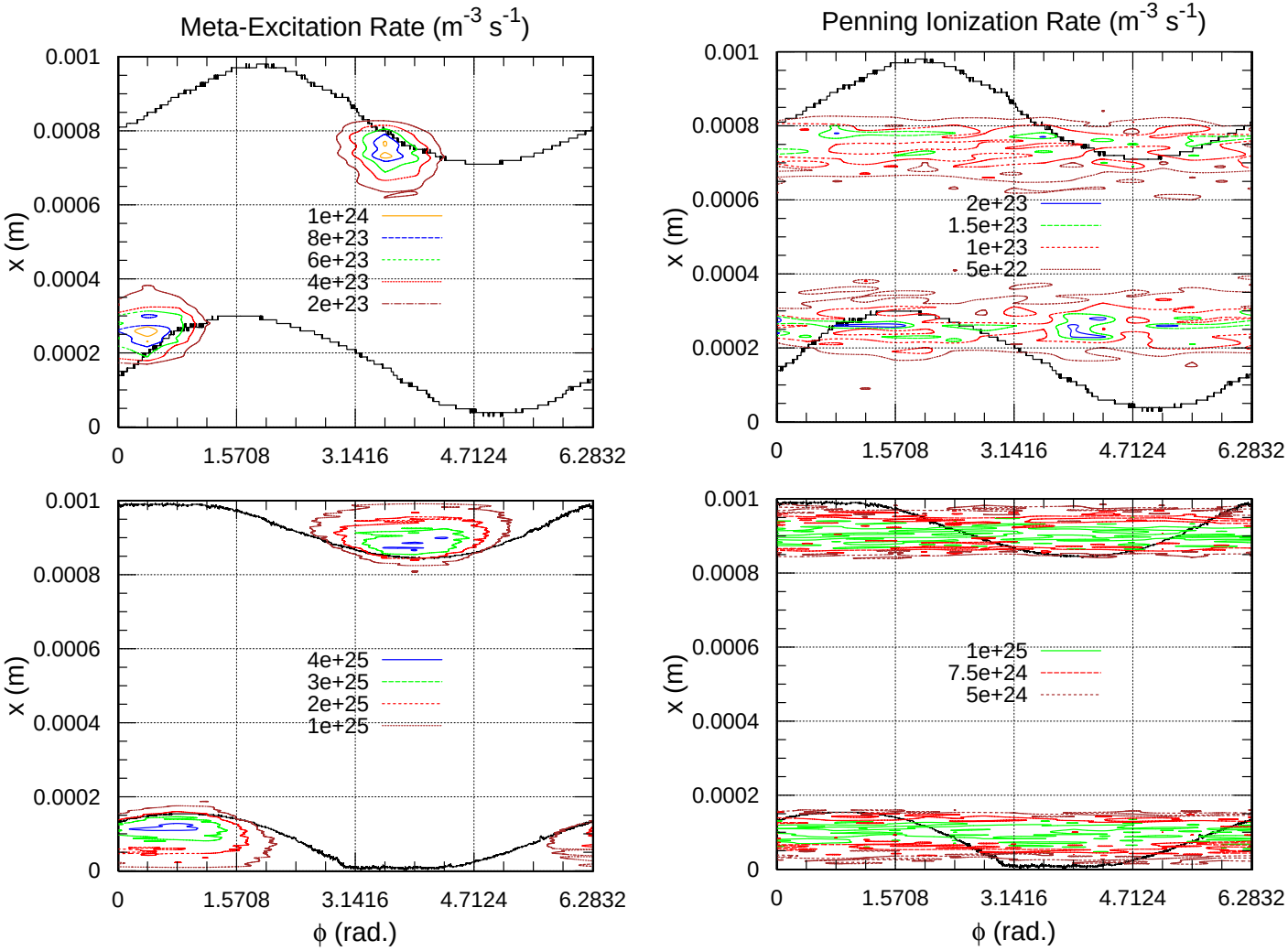
PIC SIMULATIONS OF α to γ TRANSITION IN ATMOSPHERIC PRESSURE CAPACITIVE DISCHARGES

- **400 A/m², low power α mode.**
- **2000 A/m², high power γ mode**
- **27.12 MHz, He/N_2 = 99.9/0.1**



- **From α to γ : Sheaths narrow, and excitation and ionization confined to sheaths.**

Plasma-induced crystallization of silicon nanoparticles

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The ability to form crystalline group IV nanoparticles makes plasma synthesis an attractive nanomaterials synthesis method [1]. However, temperatures that are significantly higher than the gas temperature are required for crystallization of nanoparticles. The nanoparticle heating remained a poorly understood aspect for many years. In this study, we investigated the crystallization of nanoparticles using a tandem plasma configuration, characterizing both the nanoparticles and the plasma to obtain a comprehensive understanding of nanoparticle heating in the plasma. We found that silicon nanoparticles are able to reach temperatures that are significantly higher than the gas temperature during synthesis [2].

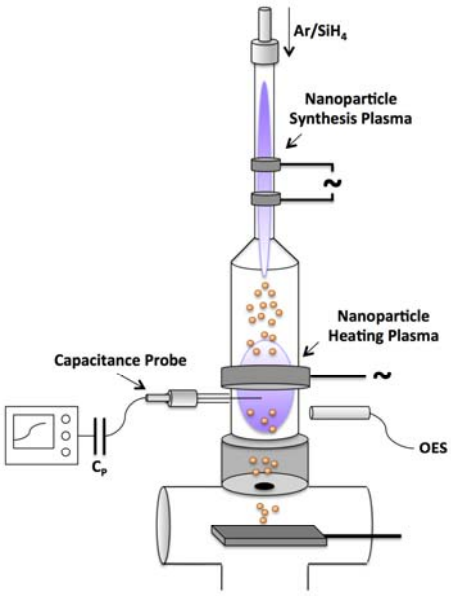

Fig. 1 – Schematic of the tandem plasma experimental setup.

First, amorphous silicon nanoparticles, 3 to 5 nm in diameter, are formed in a low-power upstream plasma. These amorphous nanoparticles are then injected directly into a separate secondary plasma which is operated with variable power, as shown schematically in Fig. 1. This decouples the synthesis and heating of the nanoparticles. *Ex-situ* characterization of the nanoparticles using x-ray diffraction (XRD), Raman spectroscopy and transmission electron microscopy (TEM) showed that crystallization occurs at a threshold power of 20 W to 40 W in the secondary plasma, depending on the nanoparticle size.

The second step is an in-depth plasma characterization of the secondary plasma to reveal the underlying plasma physics leading to nanoparticle crystallization. We performed optical emission spectroscopy (OES) to obtain the electron temperature and hydrogen density during nanoparticle crystallization. In addition, we employed a capacitive probe for ion density measurements.

The combination of the comprehensive plasma characterization and a nanoparticle heating model reveals the underlying plasma physics leading to crystallization. Here we found that the nanoparticles reach temperatures as high as 750–850 K in the secondary plasma, which is well above the gas temperature and sufficient for complete nanoparticle crystallization.

References

[1] L. Mangolini.; E. Thimsen, and U. Kortshagen, Nano Letters, **5**, 655 (2005).
[2] N.J. Kramer, R.J. Anthony, M. Mamunuru, E.S. Aydil and U.R. Kortshagen, J. Phys. D: Appl. Phys, **47**, 075202 (2014).

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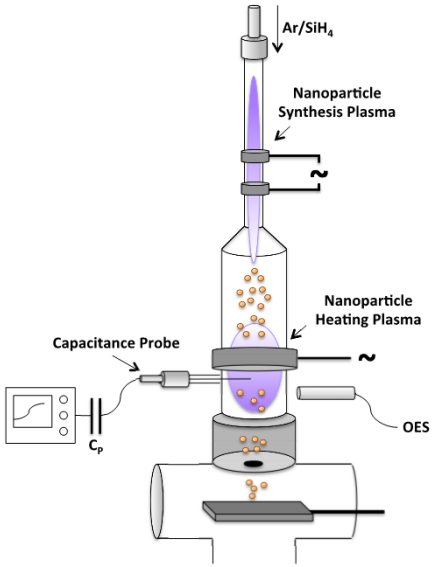
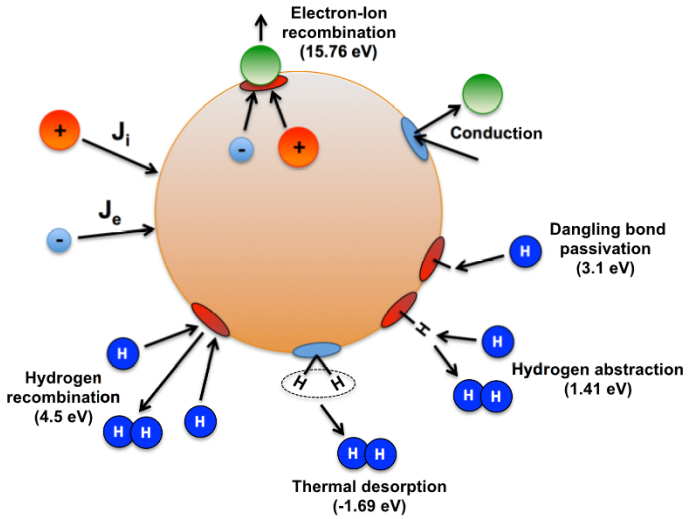
PLASMA-INDUCED CRYSTALIZATION OF SILICON NANOPARTICLES

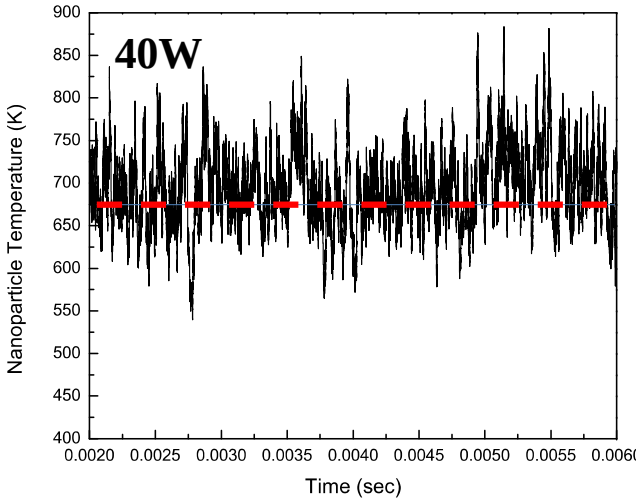
- **A combination of comprehensive plasma characterization with a nanoparticle heating model revealed the underlying plasma physics leading to crystallization of silicon nanoparticles in non-thermal plasmas.**
- **We found that the silicon nanoparticles reach temperatures as high as 750–850 K in the plasma, which is well above the gas temperature and sufficient for complete nanoparticle crystallization.**



- **Schematic of the tandem plasma setup**



- **Heating and cooling events on the nanoparticle surface**



- **Time dependent nanoparticle temperature.**

HIGHLIGHT

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