Numerical Modeling of Silicon Particle Nucleation and Growth in Chemically Reacting Argon-Silane RF Plasma

Pulkit Agarwal and Steven L. Girshick
Dept. of Mechanical Engineering, University of Minnesota, Minneapolis, MN
slg@umn.edu

We have developed a 1-D, transient numerical model of a radio frequency (RF) argon-silane plasma in which silicon particles nucleate and grow. This model self-consistently couples a plasma module, a chemistry module and an aerosol module. The plasma module solves population balance equations for electrons and ions, the electron energy equation under the assumption of a Maxwellian velocity distribution, and Poisson's equation for the electric field. In previous work, we did not model chemistry but instead assumed parameterized rates of nucleation and particle surface growth.[1-3] In the present work we calculate particle nucleation and surface growth rates using a plasma chemistry module, which treats silane dissociation and reactions of silicon hydrides containing up to two silicon atoms. The nucleation rate is equated to the rates of formation of anions containing two silicon atoms, and a heterogeneous reaction model is used to model particle surface growth. The aerosol module uses a sectional method to model particle size and charge distributions. Effects considered include particle charging, coagulation, and particle transport by neutral drag, ion drag, electric force, gravity and Brownian diffusion.

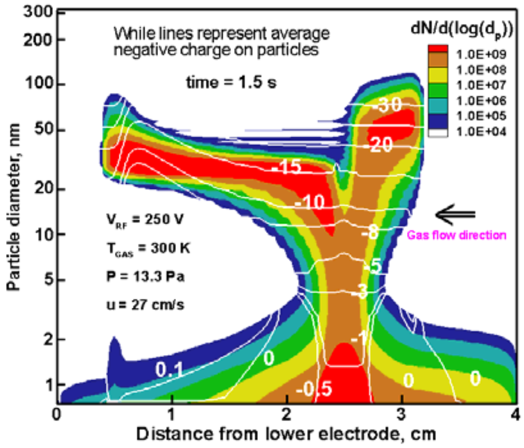


Fig. 1 – Predicted profiles over electrode gap of particle size distribution and average particle charge (white lines), 1.5 s following plasma turn-on.

Predicted particle size distributions (color contours) and average particle charge (white lines) are shown in Fig. 1 over the 4-cm gap between two parallel-plate electrodes 1.5 s following plasma turn-on. Conditions are: 250 V (amplitude) applied RF voltage at 13.56 MHz, 13.3 Pa (100 mTorr) pressure, gas velocity through the top (showerhead) electrode of 27 cm/s, and an Ar:SiH_4 ratio of 30:1.

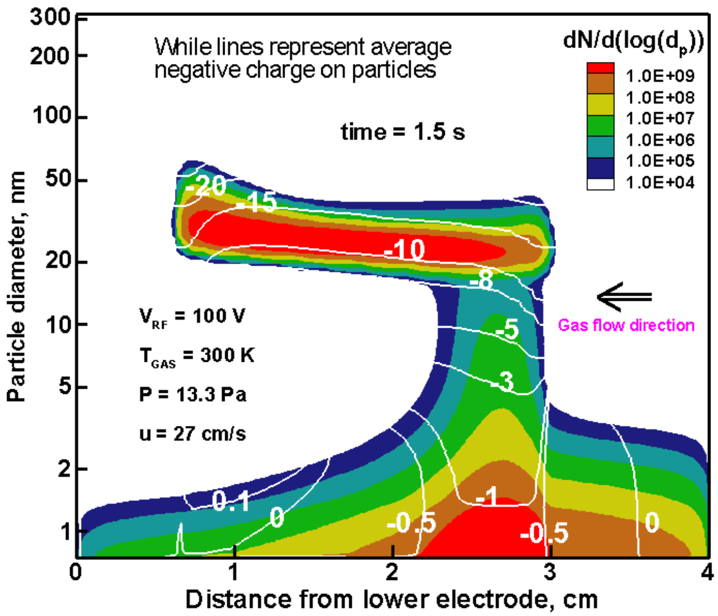
Results show the existence of spatially distinct aerosol populations, caused by the competition between neutral gas drag and ion drag. As ion drag depends not only on particle size but also on charge (which is roughly proportional to size), only the larger particles, around 50 nm, are pushed toward the upper electrode, opposite the direction of neutral drag. This creates a void in the center of the plasma, allowing fresh nucleation of very small particles to occur.

References

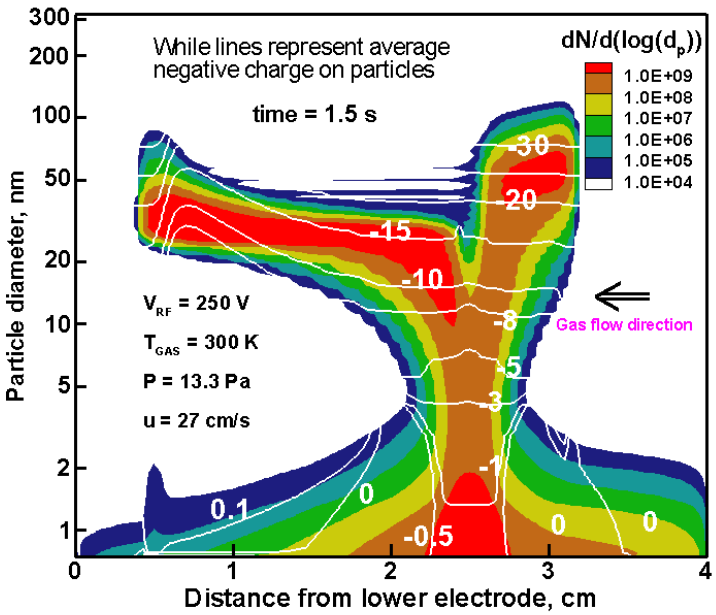
[1] S. J. Warthesen and S. L. Girshick, Plasma Chem. Plasma Process. **27**, 292 (2007).
[2] L. Ravi and S. L. Girshick, Phys. Rev. E **79**, 026408 (2009).
[3] P. Agarwal and S. L. Girshick, Plasma Sources Sci. Technol. **21**, 055023 (2012).

EFFECT OF RF VOLTAGE ON STRUCTURE OF A NANOPARTICLE CLOUD

- Numerical model includes self-consistent modules for plasma, chemistry and aerosol for a capacitively-coupled RF argon-silane plasma.
- Nanoparticles are pushed towards lower electrode by gas flow, and towards both electrodes by ion drag.
- Increasing voltage increases ion drag, enabling particles to overcome neutral drag and push sufficiently large particles towards upper electrode.



- RF voltage = 100 V



- RF voltage = 250 V