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Modelling of formation and transport of nanoparticles in silane discharges

K. De Bleecker[1], A. Bogaerts[1], W.J. Goedheer[2], R. Gijbels[1]

1. Plasmant (Dept. of Chemistry), University of Antwerp (UA), Universiteitsplein 1, 2610 Wilrijk, Belgium (e-mail: kathleen.debleecker@ua.ac.be)
2. FOM-Institute for Plasma Physics 'Rijnhuizen', P.O. Box 1207, 3430 BE Nieuwegein, The Netherlands

ABSTRACT

In this paper the behaviour of nanoparticles in a low-pressure silane discharge is studied with the use of a self-consistent one-dimensional (1D) fluid model. Nanoparticles of a given (prescribed) radius are formed in the discharge by the incorporation of a dust growth mechanism, i.e. by including a step in which large anions (typically $Si_{12}H_{25}^-$), produced in successive chemical reactions of anions with silane molecules, are transformed into particles. Several simulations with different particle radii are performed.

1. INTRODUCTION

Over the last decade, dust formation has been an important issue in many industrial applications. Besides the negative aspects of particle formation in microelectronic devices, the presence of fine dust particles in the plasma can be beneficial in certain optoelectronic applications. For example, the inclusion of nanocrystalline silicon particles in the PECVD of amorphous hydrogenated silicon (a-Si:H) thin films, results in the production of a new material, i.e. polymorphous silicon (pm-Si:H). This material proves to have superior electronic properties, and, hence is considered as a candidate for the production of high-efficiency solar cells that exhibit a good stability against light-induced defect formation. Since better management or control of the formed dust particles is required in practically all applications, a better understanding of their behaviour in the discharge is of essential importance.

In this talk we focus on the particular case of the formation and behaviour of sub-micrometer particles (ranging in size between 10 and 100 nm in diameter) in a low-pressure capacitive radio-frequency silane (SiH_4) discharge. Numerical simulations with a self-consistent 1D fluid model are used to obtain information on the nanoparticle's transport, charging and formation. A series of simulations with varying particle radius were performed to investigate their different density profile and charging. In all calculations an electrode spacing of 2.7 cm has been adopted and the results are computed for an input SiH_4 gas flow of 20 sccm, a

pressure of 40 Pa, a power of 5W, a driving frequency of 50 MHz, and a standard gas temperature of 400 K.

2. DUST NUCLEATION

Anions are generally considered to be good candidates to trigger particle formation, as they are electrostatically trapped in the plasma centre by the ambipolar potential and, therefore, have longer residence times in the discharge. In this model successive reactions of anions with silane molecules represent the main growth mechanism of particle formation. Figure 1 shows the typical density profiles of the different anions simulated in the chemistry model. Starting from SiH_3^- and SiH_2^-, two different pathways can be distinguished, leading to the formation of larger silyl ($Si_nH_{2n+1}^-$) and silylene ($Si_nH_{2n}^-$) anions, respectively [1, 2]. Note that in this model both $Si_{12}H_{25}^-$ and $Si_{12}H_{24}^-$ do not undergo further polymerization reactions, and are therefore considered as the summation of all bigger particles. The production rate of these particles will serve as the starting point of the nanoparticle formation (see below).

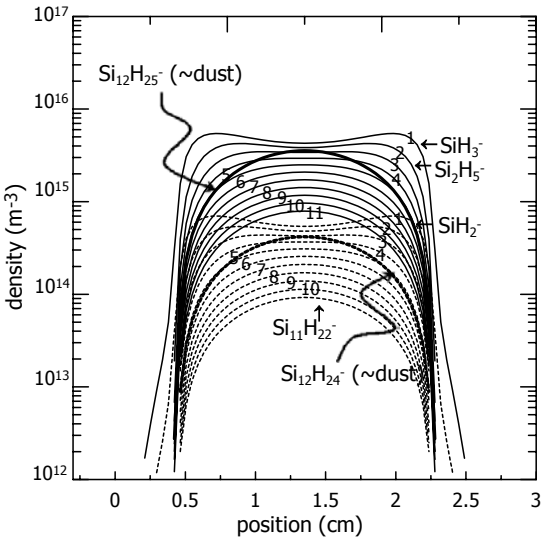

Figure 1: Calculated density profiles of anions containing up to 12 silicon atoms as a function of position in the plasma: the silyl anions ($Si_nH_{2n+1}^-$), represented by solid lines, and the silylene ($Si_nH_{2n}^-$) anions, represented by dashed lines. The number indicated on each plot specifies the number of silicon atoms.

3. NANOPARTICLE SIMULATION

The production rates of the largest species in the nucleation or chemistry model (in this case mostly $Si_{12}H_{25}^-$) are used as a source term for the production of nanoparticles of a certain prescribed radius [3]. Figure 2 shows the computed normalized density profile of the nanoparticles, at the conditions discussed above. Each plot represents a separate simulation, as the production rate of the chemistry model leads to the production of particles with a diameter of 10, 20, 30, 40, 50, 75 or 100 nm, respectively. The resulting density profile clearly greatly depends on the balance of the different forces acting on the nanoparticles: the

larger nanoparticles are accelerated by the ion drag force towards the plasma boundaries, until they begin to feel the action of the electric field. Hence, the particles are trapped in a specific region of the plasma due to the competition of the different forces acting on the nanoparticles. Note that no heating or cooling of the electrodes is considered in the present calculations, hence thermophoresis is neglected. The gravitational force is also considered to be negligible due to the small size of the particles under consideration.

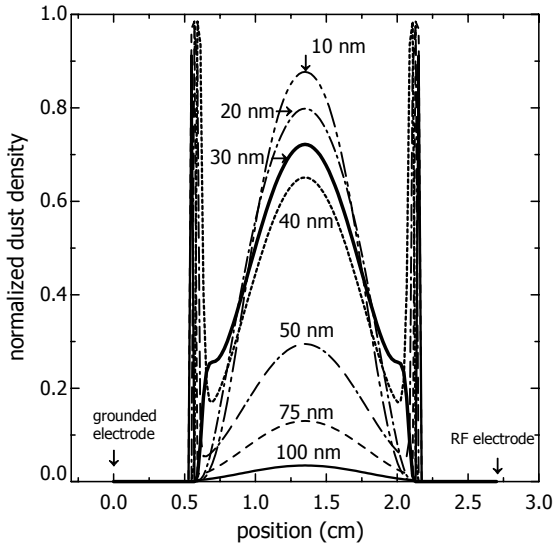

Figure 2: Calculated normalized nanoparticle densities as a function of position in the plasma. The curves of 50, 75 and 100 nm are divided by a factor 2, 4, and 10, respectively, in order to fit the data on the same figure.

The nanoparticles in the plasma generally obtain a negative charge due to the collection of plasma electrons and ions. The magnitude of the negative charge will strongly depend on the particle size and the plasma conditions. For each nanoparticle the charge distribution is obtained by means of the orbital motion limited (OML) probe theory. Figure 3 shows the computed charge collected on the nanoparticle's surface, where the charge seems to rise drastically with increasing particle size. Obviously, nanoparticles of a certain size will only be able to escape from the discharge if they are able to overcome the maximum negative charge located near the sheaths.

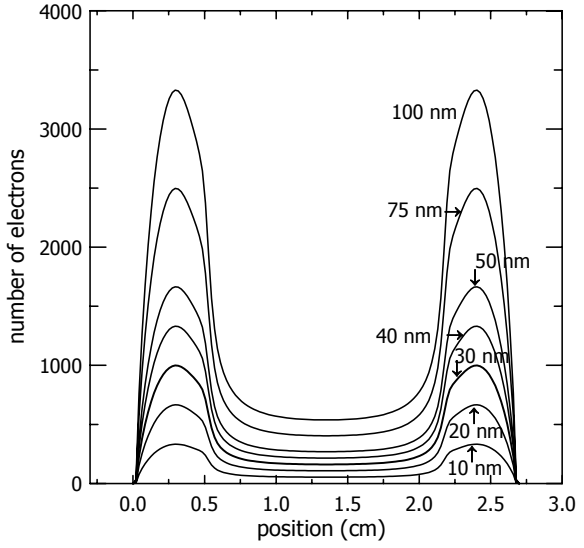

Figure 3: Calculated charge on the nanoparticles as a function of position in the plasma.

Finally, the effect of varying gas temperature on nanoparticle growth has been investigated. Multiple simulations at gas temperatures ranging between ambient temperature and 500 K have been performed. Figure 4 shows the evolution of the density of a 10 nm particle in the centre of the discharge as a function of time. The steeper rise of the density at lower gas temperatures can readily be observed, which suggests a delay in particle growth with increasing gas temperature. The same delay has also been observed in experimental setups.

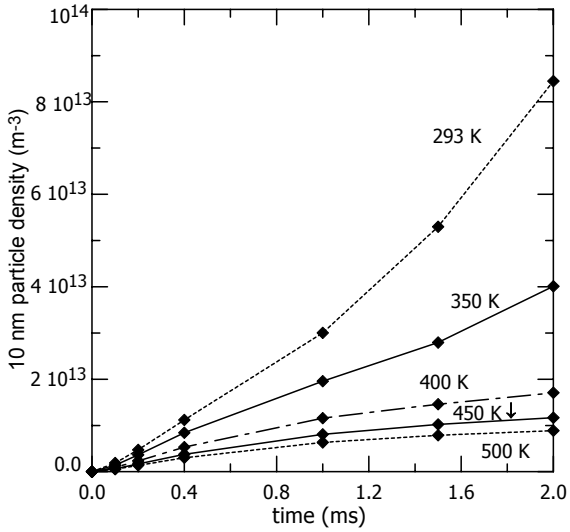

Figure 4: Predicted evolution of the 10 nm particle growth at various gas temperatures. (Note that we are mostly interested in the difference in particle growth at different gas temperatures rather than the absolute values of the number density, as the immediate transformation of particles with 12 silicon atoms to 10 nm particles in the model will probably lead to a faster build up of the dust).

4. ACKNOWLEDGMENTS

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5. REFERENCES

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