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Multiphysics modelling of nanoparticle detection / current status and collaboration sought

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Abstract: Numerical simulation of a capacitive type nanodetector is presented. The principle of operation of the detector is based on nucleation of nanoparticles in water vapor resulting in small water droplets. The droplets are fed to the capacitive type sensor which is constructed as a parallel plate capacitor filled with water. The impinging droplet creates a well in the water which modifies electrostatic energy of the capacitor and thus the capacitance. The process is modeled by electrostatic quasi 3D simulation for various terminal velocities of the droplets. Capacitance changes in the range of picofarads have been calculated from simulations. These changes are sufficient to be detected by appropriate electronics.

Keywords: nanoparticles, detection, sensor, capacitance, electrostatic energy.

1. Introduction

Nanoparticles are difficult to detect due to their small size especially with low cost equipment. The most frequently used instrument for nanoparticle separation is the Scanning Mobility Particle Sizer (SMPS) that separates the particles according to their size by charging the particles and then separating them using electrostatic forces. This is performed by a Differential Mobility Analysis unit - DMA [1]. In order to count the particles a principle of light scattering of encapsulated nanoparticles by some liquid is most frequently used. Due to the complexity of the measurement more convenient and low cost approaches are desirable.

We have recently [2, 3] presented/proposed an approach of nanoparticle counting by using a capacitive type detector that is simple in design and could lead to miniaturization and simplification of nanoparticle counting methods. The experimental system is shown in Figure 1 and consists of three parts: a nucleation/condensation chamber, a sensor and associated electronics. The principle of operation is based on subjecting the nanoparticles to water vapor that enables condensation of nanoparticles to form small water droplets. The water droplets are further fed to a capacitive type nanodetector. The detector is designed as a parallel plate capacitor filled with water with an additional bottom dielectric layer used for AC coupling the detector to electronics. At impaction of water droplets with water filled detector the capacitance of the detector changes which is detected by suitable low noise electronics. This paper presents numerical simulation of operation of a nanoparticle counter and calculation of capacitance change during droplet impaction.

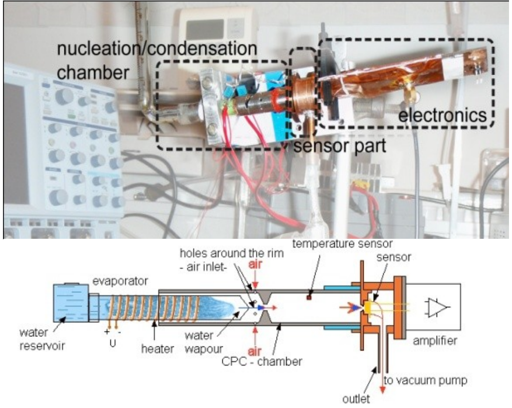

Figure 1. Experimental system for nanoparticle counting by condensation of nanoparticles and formation of water droplets which are further impinging onto a capacitive type detector that changes capacitance at impaction of water droplets.

2. The sensor

The sensor is constructed as a parallel plate capacitor with perforated top electrode as shown in Figure 2. A mesh used for TEM microscopy was used in the experiment. The area of the openings is 80x80 μm and the thickness of the mesh is 20 μm. Figure 2 presents one of the 9 cells that are forming the active area of the detector. Between the top and the bottom electrode is a thin dielectric layer (made of kapton) used to AC couple the detector to electronics. Originally there is air between the kapton and the top electrode. However, as soon as the system starts to operate, the water droplets fill the detector with water. The thickness of this layer is about 100 µm.

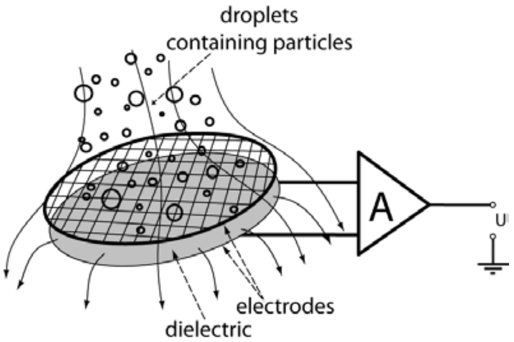

Figure 2. Capacitive type sensor with a perforated top electrode allowing water droplet impingement onto the water filled sensor.

3. Numerical simulation of detector operation

Quasi-3D numerical simulations (by assuming rotational simmetry) of a single droplet impinging onto the water filled sensor were performed. Figure 3 shows a cross-section of a simulated structure. The formation of a well in the water by the droplet was not simulated but reconstructed from high speed videos of water droplets falling into the water. Electrostatic solution of a problem was sought by applying suitable boundary conditions to the edges and electrodes. Three different cases of droplet terminal velocity were studied. In case the droplet impinges onto the water filled sensor with larger terminal velocity it creates a deeper well resulting in larger change in capacitance. Figure 4 shows results of numerical simulation of electric field distributtion (and equipotential lines) for three different terminal velocities at maximal well formation. Figure 5 presents calculated values of capacance through evaluation of electrostatic energy for 25 different simulation steps representing different time steps.

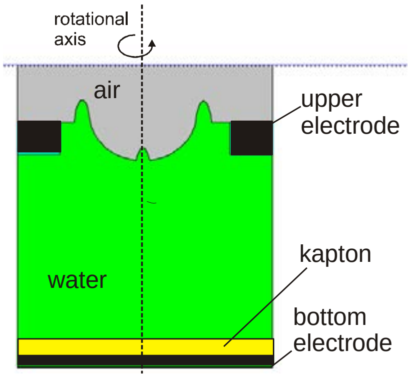

Figure 3. Cross-section of simulated structure with constitutive parts. Rotational symmetry was used for quasi 3D simulation.

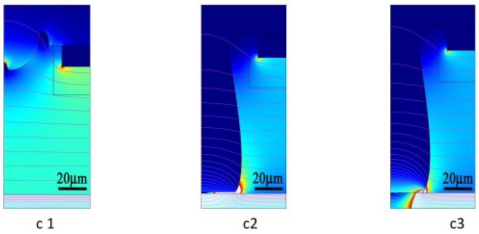

Figure 4. Numerical simulation results for three different terminal velocities of the droplet forming different depths of the well.

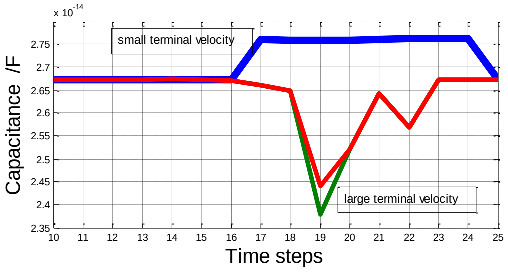

Figure 5. Capacitance change for 25 simulated steps of droplet impingement for three different droplet terminal velocities.

4. Discussion

Largest change of capacitance is obtained at the deepest well formation (cases c1, c2 and c3 in figure 4). The largest change of capacitance for the current design are of orders of picofarads which is sufficient to be measured by low noise electronics. It is interesting to note that at low terminal velocities – when the well is small compared to cases of larger terminal velocities – the capacitance increases instead of decreases as in other cases. This has been attributed to the effect of larger inhomogenities that appear around the top electrodes which increase the electrostatic energy and thus the capacitance. In case of larger terminal velocities the capacitance decreases due to reduced volume of substance between the electrodes with high permittivity (water has relative dielectric constant about 80 and air 1). This results in a reduction of capacitance. The largest energy content is in the kapton layer – a thin dielectric (shown in Figure 3) used to DC uncouple the detector. By further thinning this layer a larger change of capacitance could be obtained. However, this also increases the total capacitance of the detector which is not advantageous.

5. Conclusions

Numerical simulation of operation of a capacitive type nanodetector has been performed. It is based on detection of change of capacitance during water droplet impaction onto the water filled capacitance sensor. The simulations have proven the detection principle as well as presented some details of electrostatic energy change during formation of a well in the water filled detector which could lead to further improvements of the detector design. The movement of droplets and formation of a well during droplet impingement onto the water filled sensor was not simulated. This could be a frame for future investigations in which collaboration with researchers with expertise in water droplet deformations at impaction would be needed.

6. References

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