COMSOL Modeling of Self-Limiting Electrospray Deposition

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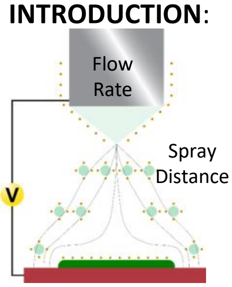
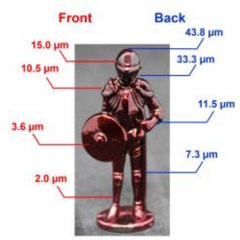
INTRODUCTION:

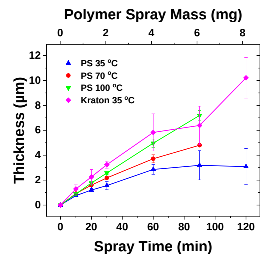


Model of SLED film formation

Electrospray Deposition (ESD) is a process by which a solution is passed through a charged capillary, causing the solution to form a Taylor cone and break up into small droplets through a series of "Coulomb fissions." The charge build-up on the spray target eventually causes the spray to deflect from coated areas, causing the coating to spread out, allowing it to coat complex 3D structures. This is known as self-limiting ESD (SLED). Polystyrene (PS) sprayed from 2-Butanone under SLED mode was simulated in this study.



Film thicknesses recorded on SLED coated knight [1]

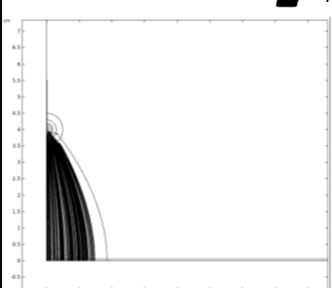


Central thickness of PS and Kraton Samples at various spray times

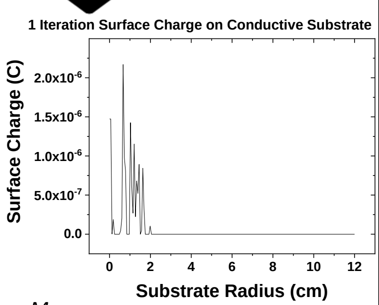
COMPUTATIONAL METHODS:

This set-up was completed using a 2D-axisymmetric model and electrostatics module. Surface charge density was applied to line above substrate line, representing film charge. Ground was used on the bottom line representing the 2D conductive plate substrate. Electric potential was used at rectangle on left representing a charged needle. The particle trace found for the surface charge density function for the following iteration and LiveLink was used to allow a MATLAB wrapper function to run the simulation continuously, modeling the charge and film build-up over time.

Particle Trace



COMSOL Model of geometry used and resulting particle trace of SLED model

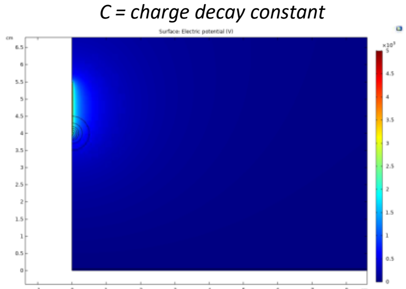


Surface Charge Density after one iteration of particle trace

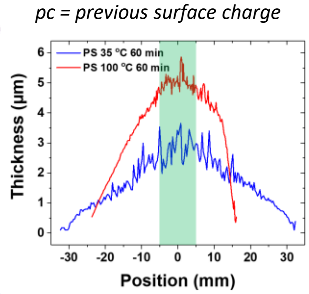
Charge Map

Film deposition was compared to physical models to find proper charge decay constant for polystyrene (PS), which governed the surface charge using the following equation: $\mathbf{y = pc(1-e^{C/t}*dt) + cc}$

y = charge array
cc = new charge added
C = charge decay constant
t = total film thickness
dt = time step
pc = previous surface charge



Electric potential field from COMSOL simulation

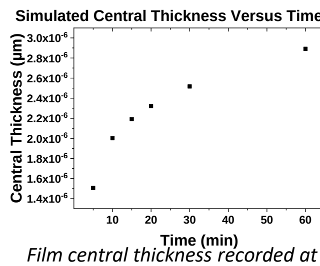


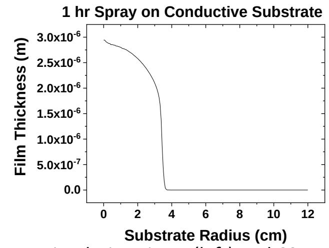
Physical film thickness found across center of PS samples

RESULTS:

Simulation runs resulted in similar thickness readings and runs in comparison to physical models of PS ESD. The best thickness thus far resulted from a charge decay of 1.4*10^-5, and a charge per particle value of 1*10^-8.

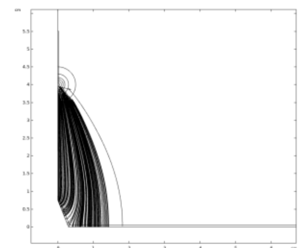
This central thickness was 2.8911*10^-6m while physically it should have been 2.760*10^-6m, which is within 5% error. The spread also matched relatively well. This was a good starting point, and will lead to a more accurate decay constant for PS.



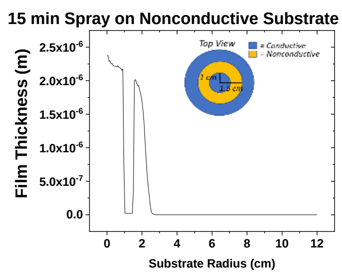


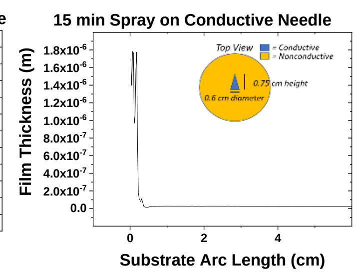
*Film central thickness recorded at different simulation times (left) and 60 minutes (right) of simulated spray with a charge decay of 1.4*10^-5 and charge per particle value of 1*10^-8*

This charge decay constant was then used to model two different simulations. The first was a flat substrate with a nonconductive strip across it where the charge decay would not occur. The second was a needle geometry shown to the right with the surrounding surface being nonconductive.



COMSOL Model of Needle geometry and resulting particle trace





Film thickness deposited in 15 minutes simulated spray time on a substrate with a nonconductive strip from 1-1.5cm radius (left) and on a substrate with a conductive needle from 0-0.3cm radius and surrounding nonconductive area (right)

CONCLUSIONS:

The SLED process can allow complex 3D structures to be coated evenly and can allow complex nanostructures to be added onto a surface for additional surface properties. Advantages of SLED also include not needing to move the spray needle while coating, a high coating efficiency, and a cheaper means of creating a complex nanostructured coating.

This method is approaching charge decay and SLED parameters for PS. It can be used for different materials and different geometries and can allow manufacturers to determine coating thickness and efficiency under different conditions, allowing ESD to be a more viable manufacturing tool. From here, it would be important to investigate possible physical phenomena resulting in spiked surface in physical models missing from simulation.

REFERENCES:

1. Lei, L., Kovacevich, D. A., Nitzsche, M. P., Ryu, J., Al-Marzoki, K., Rodriguez, G., Klein, L. C., Jitianu, A., Singer, J. P., Obtaining Thickness-Limited Electrospray Deposition for 3D Coating, ACS Applied Materials & Interfaces, 10(13), 11175-11188, (2018)
2. Merrill, M., Pogue, W. R., III, Baucom, J., Electrospray Ionization of Polymers: Evaporation, Drop Fission, and Deposited Particle Morphology, J. Micro Nano-Manuf., 3, No. 011003, (2015)