A Model for Finite Non-Equilibrium Electrolyte Solutions: Mapping the Electric Double Layer

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Electric Double Layer Theory

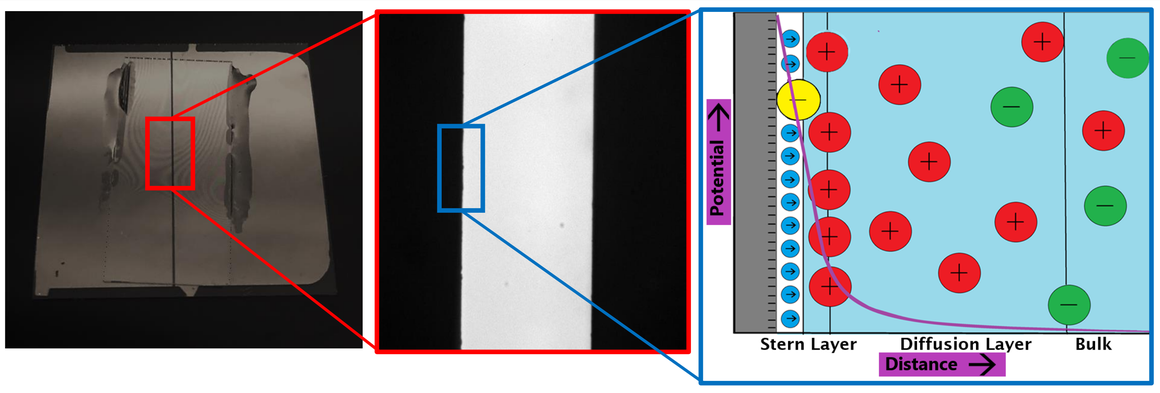


Figure 1 (Left) 25x25 mm microfluidic double electrode cell sealed with UV-glue. Nickel-Chromium metal electrodes are 50 nm in height and 175 µm apart and 20 mm long.
Figure 2 (Center) 40x magnification of the 175 µm gap between the electrodes. The 20 nm particles in solution are too small to be seen by light-waves, and must be analyzed via fluorescence super-resolution microscopy.
Figure 3 (Right) A brief overview of Electric Double Layer (EDL) theory [1]. At equilibrium, electrolytes in solution will arrange on or near a charged surface according to the electronic potential applied [2]. In the Bulk region, or with zero potential applied, the solution is assumed to homogenously even throughout.

Double Electrode Side-view

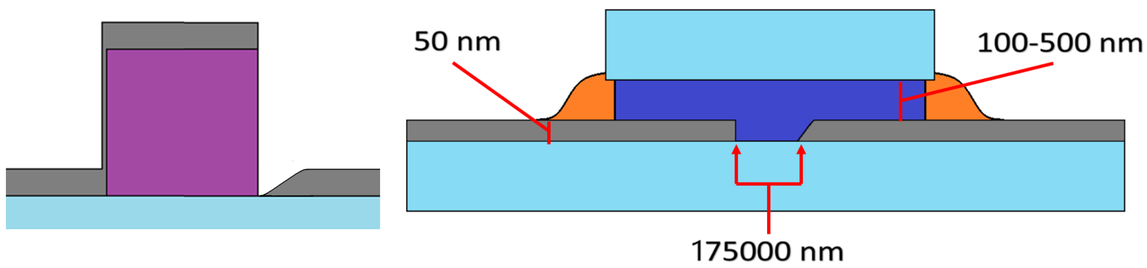


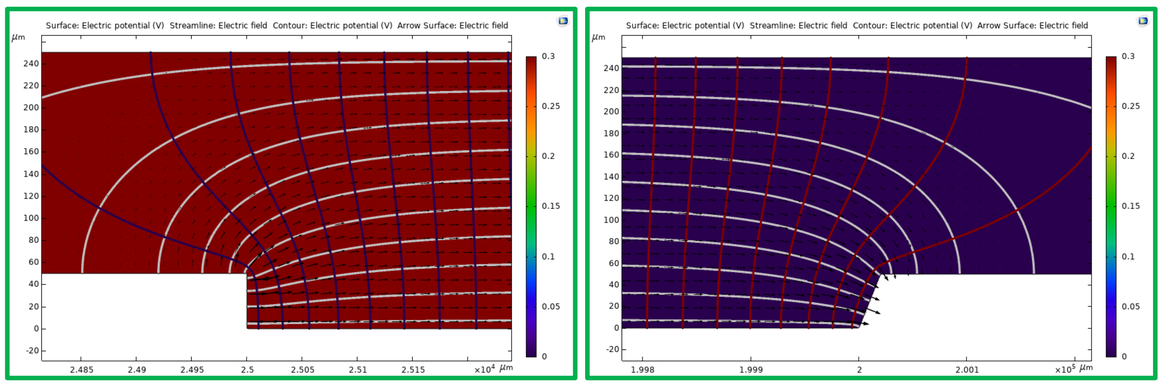
Figure 4 (Left) When layering metal onto larger photoresist structures, penumbra effects must be taken into account. The "shadowed" surface will be angled, displacing the top surface by 20 nm.
Figure 5 (Right) An exaggerated-scale diagram. In contrast to a top-down view, a side view shows a more realistic view of the field effects in solution.

COMSOL Simulation Criteria

All COMSOL calculations are 2D Stationary, using the Electrostatics Interface of the AC/DC Module. The left electrode is set at 0.3V and the right electrode is ground, the material medium is Water, and the channel height set to 250 nm.

Figure 6 (Below-Top) Full-scale simulation.
Figure 7 (Below-Bottom) 1/100 scale of the 175 µm gap.
Note: Electrodes are still full-scale

Comparing the Electric Fields



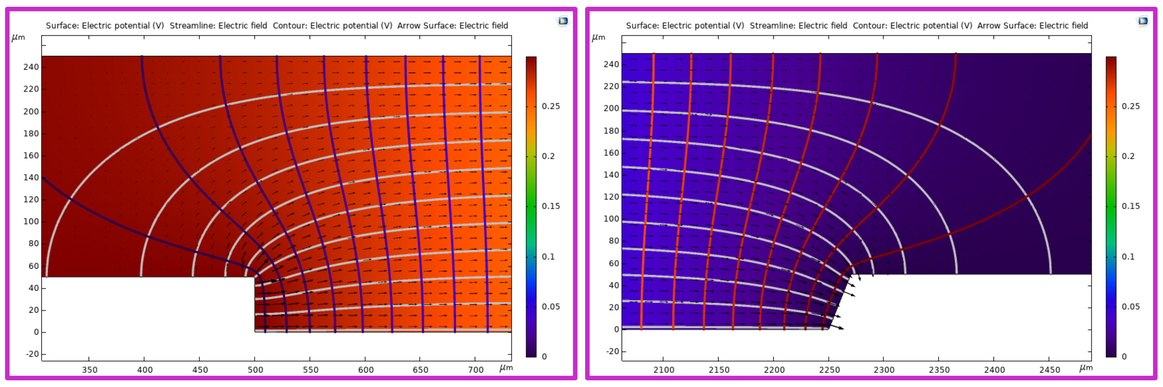


Figure 8 & 9 (Top Set) Electrode surfaces expanded from the green boxes on the full-scale simulation. The voltage gradient is accurate, but effectively useless. Contour lines for the voltage and Streamlines for the field are far more reliable in showing the exact nature of the field along the electrode, while arrows help highlight the magnitude.
Figure 10 & 11 (Bottom Set) Electrode surfaces from the 1/100 scale simulation. While the voltage gradient is exaggerated, the contour lines, streamlines, and arrow magnitude are near-perfect matches to the full-scale model.

Conclusions and Future Goals

After reducing the boundaries of our simulation by 1/100, but without reducing the electrode surface geometry, we can safely shift calculation runtime away from the large simplistic volume of the full-scale model and instead enhance calculations on the electrode-solution interface. Any geometry/meshing issues due to vastly different dimensions are solved in our reduced model.

Our next goal is to adapt this into the Particle-Tracing Interface in order to simulate our particles interaction with the Electric Double Layer in our microfluidic cell.

Acknowledgements and References

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1) Brown, M. A, et al, "Determination of Surface Potential and Electrical Double-Layer Structure at the Aqueous Electrolyte-Nanoparticle Interface" in Physical Review X, Vol.6-1 (2016)
2) O. Stern "Zur Theorie Der Elektrolytischen Doppelschicht" Z. Elektrochem., 30, p. 508 (1924)
3) Carlson C, Sweeney N, Nasse M, Woehl J "The corral trap: fabrication and software development" in Proceedings of the SPIE, Vol 7571, pg. 757108-757108-6 (2010)