Space-Charge Limited Current Calculations in Nanowires

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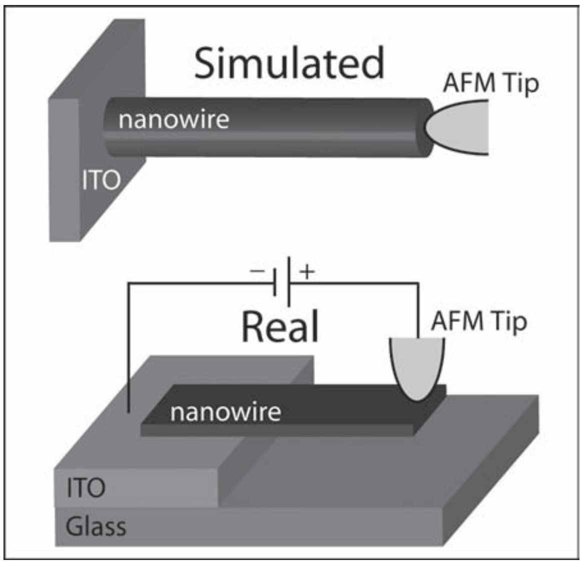

Figure 1: (top) The geometry of existing numerical models for space-charge limited current through a nanowire. (bottom) The geometry of AFM experiments on which space-charge limited currents are measured.

Abstract and Introduction:

Existing models of a space-charge limited current through a single polymer nanowire do not agree with experimental data from conductive-atomic force microscopy measurements. A better theoretical understanding of space-charge limited transport in these polymer nanowires [1] would allow for quantitative carrier mobility measurements [2]. Our hypothesis was that the disagreement between existing models and experiments was due to differences in the geometry. In this work we developed a numerical model that has a geometry conforming much more closely to that found in experimental measurements (see Figure 1). Our results suggest that the discrepancy between our models and experiments cannot be explained by this difference in geometry.

Procedure:

We used two coupled differential equations to simulate charge transport in our model: the drift-diffusion equation and the Poisson equation. The drift-diffusion equation describes how charge-carriers move through an electric field and in response to charge density gradients, while the Poisson equation describes how the electric field is affected by the charge-carriers.

We used COMSOL Multiphysics 3.5a to solve this coupled system of equations in a variety of geometries. This software solves differential equations by breaking up the geometry into smaller pieces and finding self-consistent solutions in each piece. This method is called the finite element method.

Our model development was centered on constructing a realistic geometry for the simulation. Control geometries were used in order to test that the model could reproduce understood scenarios such as the plane-parallel electrode case. Then, while only changing one element of the geometry at a time, more complicated cases (geometries) could be solved.

Results:

Figure 2 shows simulation results for the most experimentally conformal geometry we produced. The current density is much higher along the corners of the nanowire near the injection point, and then funnels towards the center of the nanowire near the extraction surface.

Figure 3 shows current-density voltage curves from an AFM experiment (circles) and our simulation (squares). The current density is dependant on the square of the injection voltage for both the experiment and the updated simulation, strongly suggesting a space-charge limited current.

Figure 4 shows current density-transport distance curves from an AFM experiment (circles), original simulation (triangles), and updated simulation (squares). Both of the simulated results show an inverse-square relationship between current density and charge-carrier transport distance. This is much different than the sub-linear dependence on length that the experimental results show.

Discussion:

It is unclear why the current density is higher at the corners in the nanowire in Figure 2. We speculate that this may not be a physical phenomenon, but rather an artifact in the simulation. This feature has been found in both the updated geometry model and in original simulations. Further investigation is required to understand the origin of this feature, and whether it effects our results for total current density.

The dependence of current density on the square of the voltage suggests that both the simulated and experimental currents are space-charge limited (see Equation 1). There is still a lack of agreement between the experimental results from the single nanowire space-charge limited current experiment and the theoretical results from the model, even after the model geometry was made to better match the conductive-atomic force microscopy experiment. Both the original model and the updated model show a length dependence on the current density of L^{-2}. This suggests that the orientation of the atomic force microscope tip does not affect the current density's length dependence.

Conclusion:

Space-charge limited current measurements have been made in the past in order to measure the charge-carrier mobility of a single semiconducting polymer nanowire [2]. The simulations that were run in parallel to this experiment did not yield results that agreed with the experimental results. It was hypothesized that this lack of agreement was due to the model geometry not being realistic enough. We have developed a new model that reorients the atomic force microscope tip to touch the nanowire on the side of the wire instead of the end, and changes its shape from cylindrical to prism shaped.

Once the geometry was updated we verified that our model still produced a quadratic relationship between current density and voltage. This is evidence that the current remains space-charge limited. The length dependence of the current density was found to be L^{-2}. This relationship is very similar to the current density-length relationship that was found in the original model. From these results we conclude that neither the orientation of the atomic force microscope tip on the nanowire, nor the exact shape of the nanowire significantly affect the charge transport characteristics.

Further modeling of alternate geometries and investigation of the experimental conditions are required in order to explain the present discrepancy between our experiment and models.

Acknowledgements:

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References:

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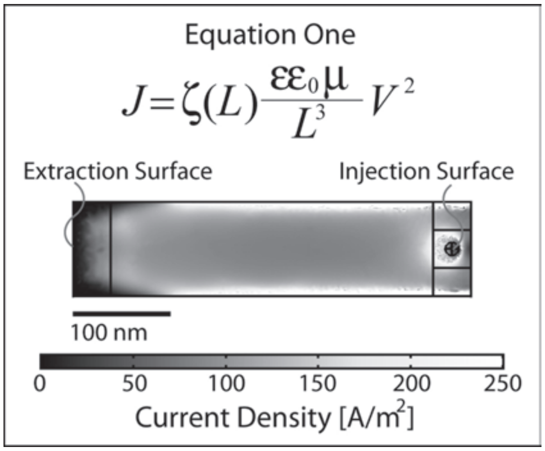

Figure 2: (top) The generalized equation for describing a space-charge limited current [3], where J is current density, ζ(L) is a geometry dependent function of length, $\varepsilon\varepsilon_0$ is the permittivity, μ is the charge-carrier mobility, V is injection voltage, and L is transport distance (wire length). (bottom) The solution of the updated model, showing current density.

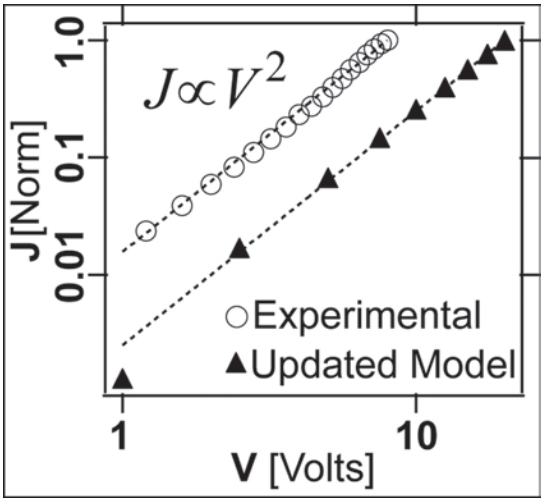

Figure 3: Current density versus injection voltage, with the experimental data (open circles), and the updated model data (closed triangles).

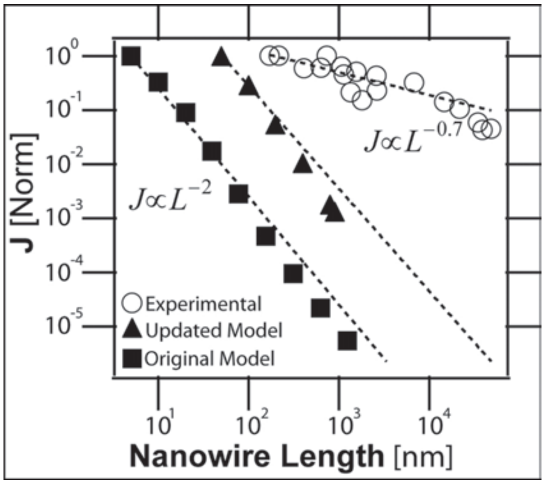

Figure 4: Current density versus wire length, with the experimental data (open circles), the updated model data (closed triangles), and the original model data (closed squares).