CALIFORNIA SCIENCE & ENGINEERING FAIR
2018 PROJECT SUMMARY

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Project Number
38424

Project Title

Gossamer: A Monte Carlo Simulator for the Optimal Design of Nanowire Networks for Transparent Electrode Applications

Abstract

Objectives/Goals

I have developed a simulator to optimize the performance of a class of electrically conductive, transparent and flexible thin films. Such materials are needed to construct components such as touchscreens and solar panels that are non-rigid and shape-conformable.

I focus on films manufactured using "solution-processing" which creates random metal nanowire (MNW) networks. Large-scale experimental characterization of the resulting sample-to-sample variability of film properties is costly and time-consuming. Gossamer, the MC simulator I developed, responds to this challenge, allowing scientists to separate systematic effects of controllable manufacturing parameters, from statistical variability.

Methods/Materials

I wrote Gossamer in Java and it consists of three modules: (a) a geometry engine which generates a random MNW collection, computes their intersections and creates a list of MNW segments, (b) a network analyzer which identifies connected clusters of MNW segments using depth-first search, and (c) a circuit solver which computes the overall resistance of the network. I used Python for post-processing and visualization.

Results

I demonstrate three applications of Gossamer: (i) characterize current hotspots within the film which cannot be explored experimentally (ii) compute film resistance as a function of wire length (Le), diameter (Di) and areal wire mass density (phi_md), and (iii) optimize film conductivity under different tradeoff conditions (e.g., Le vs. Di) subject to constant phi_md constraints.

Key findings include: (a) when film resistance is plotted as a function of phi_md, the data falls on a nearly-universal dimension-independent L-shaped curve, which correlates well with experimental data, published recently (2015) by Lagrange and Langley (b) for each choice of MNW mass density, an optimal choice of wire dimensions exists for minimizing film resistance.

Conclusions/Discussion

I developed a physics-based simulator to model the resistance and internal state of a class of conductive and transparent nanowire-based films, validated it against recently published experimental data and used it to compute geometrical parameters that optimize overall film conductance, under constant mass constraints.

Summary Statement

Gossamer, my MC simulator, helps accelerate the ongoing search for transparent conductive materials which are needed for the construction of a wide range of emerging large-area and flexible electronic devices.

Help Received

I developed the code and performed the simulations and analysis on my own. I would like to thank my mentor for discussing the current experimental literature and pointing out outstanding challenges in the field. I would like to thank my school math teacher for helpful discussions and encouragement.