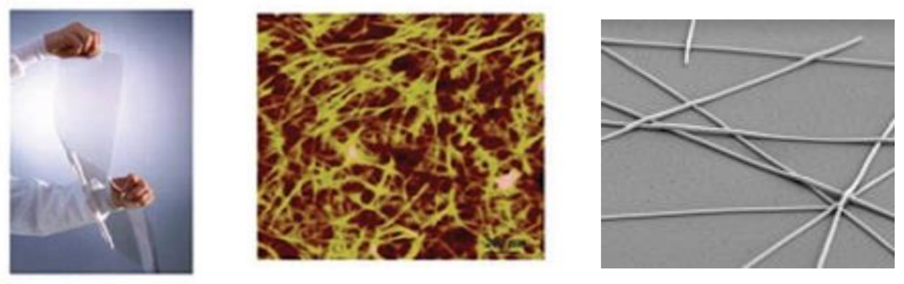
Computational Study of Random Nanowire Networks: Optimization of Conductivity through Orientation

1) Background

- Products such as touch screens, LCD displays, and solar panels use transparent conductors.
- Need high transparency and conductivity.
- Currently made mainly using ITO (indium tin oxide).
- ITO is expensive, brittle, difficult to make, and in short supply.

Is There a Better Way?



- Alternatives: graphene films, CNT dispersions, metal nanostructures.
- Random metal nanowire networks have high potential; still do not match ITO.
- **Problem: Increase conductivity for given transparency (corresponds to amount material used).**
- Computational model useful for this approach.

Objectives:

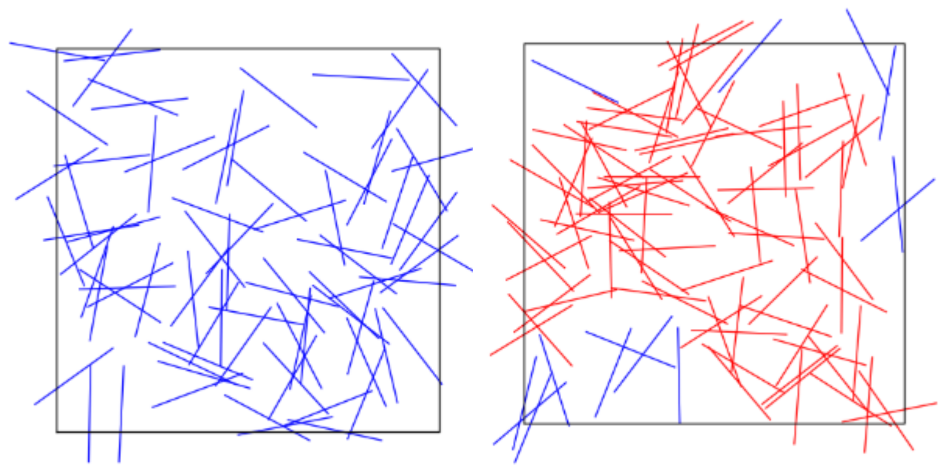
1) Develop computational model for conductivity of metal nanowire networks.

2) Use model to find ways to increase performance.

2) Computational Methods

Computational model is split into two main portions: Generation of random networks and Calculation of conductivity of networks.

- **Network generator** creates line segments in plane with three random values: x-coordinate, y-coordinate, orientation θ.
- Intersections found using algebra and segment length.
- Clustering analysis performed to see if path exists across the sample; shows if network has zero or non-zero conductivity.



Zero conductivity — *Non-zero conductivity*

- **Conductivity calculator:** Network has two types of resistors: resistance of wires (R_{rod}), and resistance of junctions between rods (R_J).
  - With metal nanowires, $R_J \gg R_{rod}$ [1].
  - R_{rod} calculated using resistivity of silver, distance between nodes, rod radius.
  - Rod dimensions taken from commercially available nanowires [2].
  - R_J assumed to be constant; this assumption has been proven valid [1].

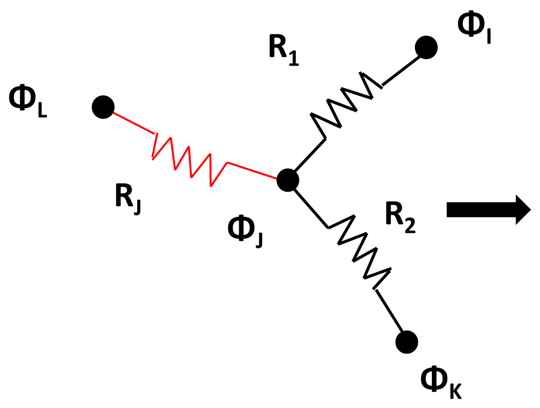
2) Methods Continued

- Finding network conductivity requires voltages at each node: need one equation per node
- Equations obtained using **Kirchhoff's Junction Law**:
  - Nodes have two wire, one junction resistor.
  - Applying **Ohm's Law** (ΔV=IR) and **Kirchhoff's Junction Law** to example on right gives:
- Equations for every node are assembled into matrix equation of form:

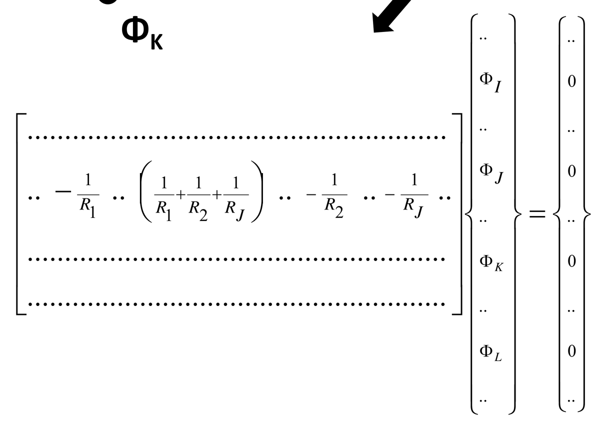
$$[A]\{\Phi\} = \{J\}$$

Where [A] contains conductances, {Φ} contains voltages, {J} contains currents

- Voltage applied left to right; solve matrix equation for {Φ} at each node
- Sum total current across boundaries; calculate conductivity from **Ohm's Law.**

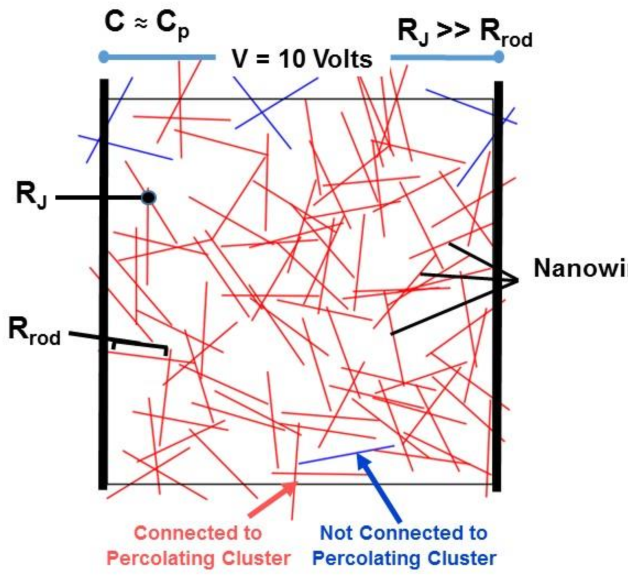


$$\frac{(\Phi_J - \Phi_I)}{R_1} + \frac{(\Phi_J - \Phi_K)}{R_2} + \frac{(\Phi_J - \Phi_L)}{R_J} = 0$$

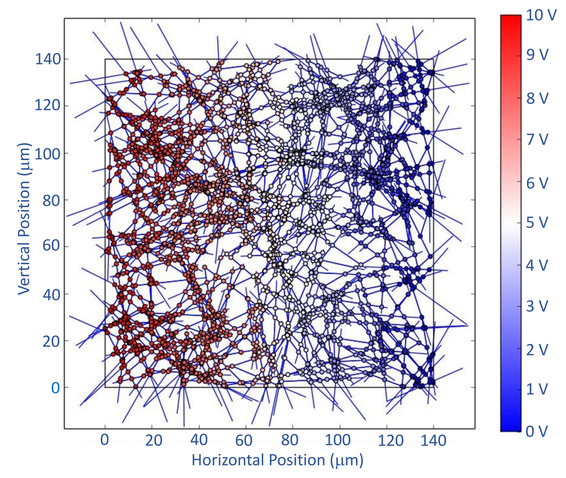


Challenges:

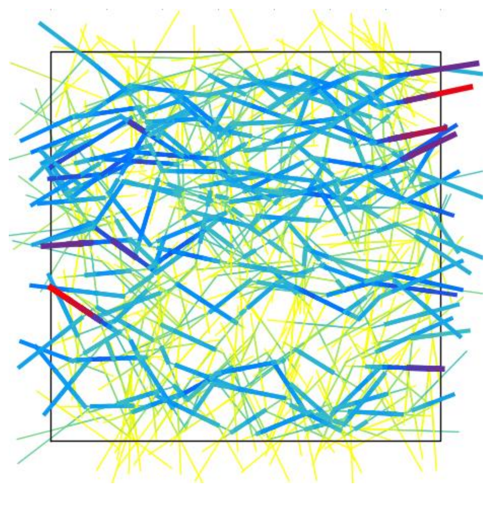
- **Large System Size:** [A] up to $(60{,}000)^2$ = **3.6 billion** floating point entries, ~ **27 GB RAM!**
- **Solution:** Optimize junction numbering and storage. Reduces RAM requirement to **<0.1 GB**
- **Large # of Calculations:** > **72 trillion** FLOP for a $(60{,}000)^2$ matrix: >**27 minutes** of clock time.
- **Solution: Minimize bandwidth**. Use **Cholesky decomposition** rather than **LU decomposition** to solve matrix equation. Reduces time to **~4 minutes per trial.**
- **Singular Matrices** arise for samples with disconnected clusters.
- **Solution:** Connect each node to "ground" through high resistance. **All nodes are connected but conductivity is not appreciably impacted.** Similar method used to apply boundary voltage.



Sample generated by program, annotated with discussed details



Color shows nodal voltages. Voltage decreases linearly across sample



Color and width of segment shows amount of current. (Red/blue is high; yellow is low)

3) Validation of Model

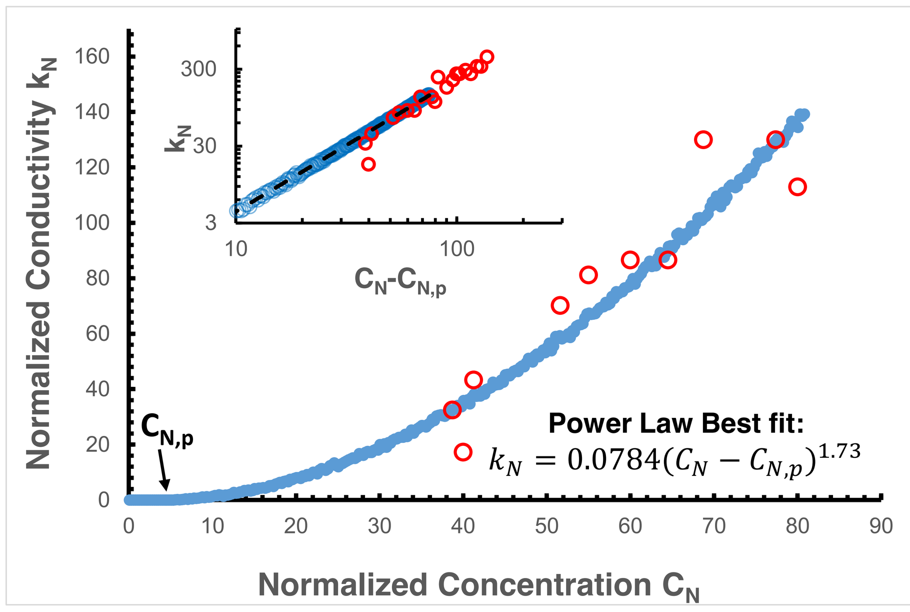
- Normalize conductivity **k** by inverse junction resistance $1/R_J$, since R_J dominates resistance.

$$k_N = k \cdot R_J$$

- Concentration **C** (total wire length divided by area) normalized by inverse piece length.

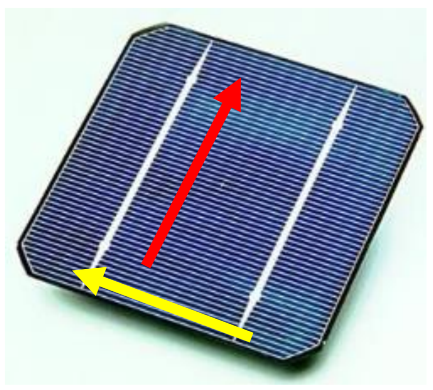
$$C_N = C^*l$$

- Generalizes results for all R_J and all rod lengths [3].



- Critical concentration for onset of conductivity marked.
- Experimental data from [1] on silver nanowire networks plotted in red; shows good fit with simulation curve.
- A power law relationship is observed, with critical exponent of 1.73. Agrees well with published results identifying critical exponent of 1.75. [1]
- **Simulation accuracy confirmed: can be used to study new variables.**
- Power-law relation implies varying length can have effect. Has been verified with model: **varying length keeping average constant increases conductivity**.

4) Optimization via Orientation

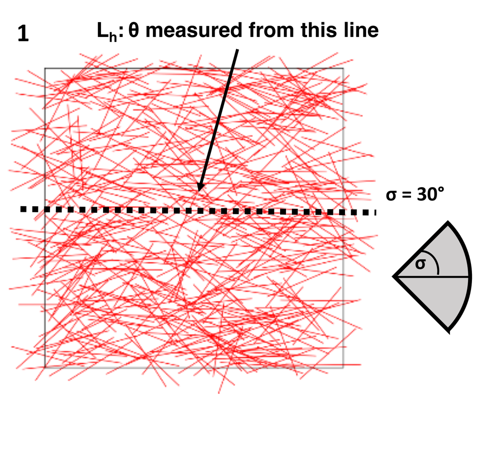


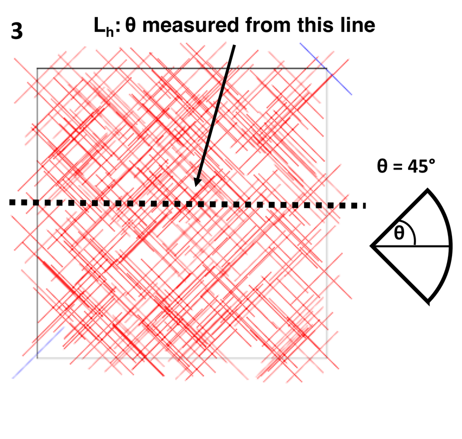
- Many applications of transparent conductors need current flow in single direction.
- Could restricting rod orientation be beneficial?
- Orientation not obviously beneficial; extreme alignment bad.

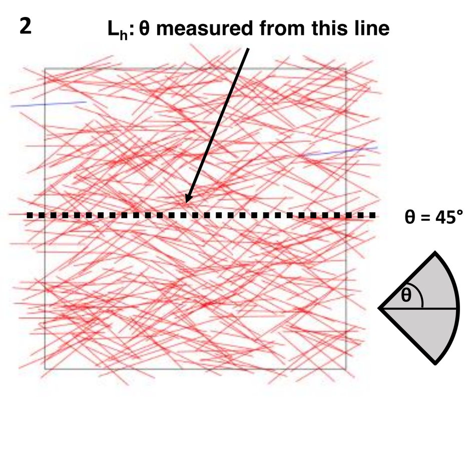
Precise physical experiments difficult; computational model allows systematic exploration.

Three distributions of varying degrees of randomness tested. Samples shown below:

1. Normal distribution, Standard deviation: σ.
2. Orientation in range (-θ, θ); $\theta = \sqrt{3}\sigma$
3. Orientation in range [-θ] ∪ [θ]; $\theta = \sigma$



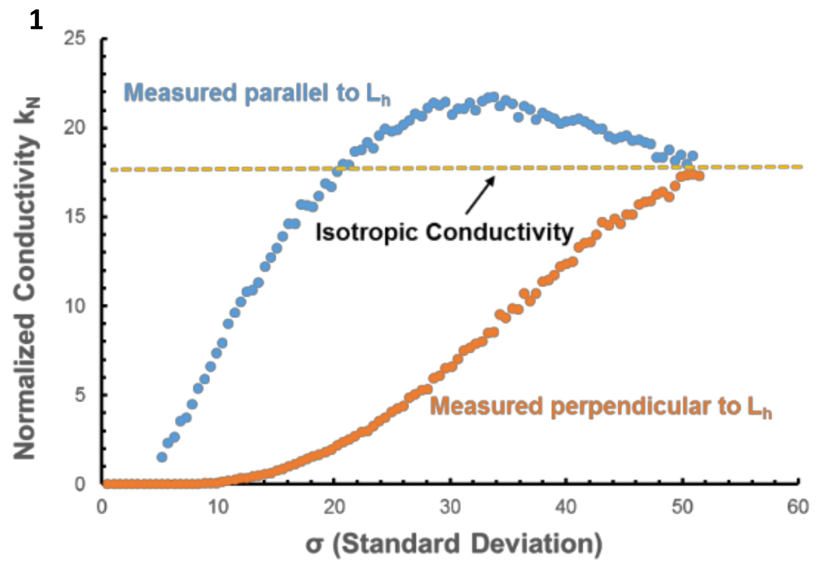




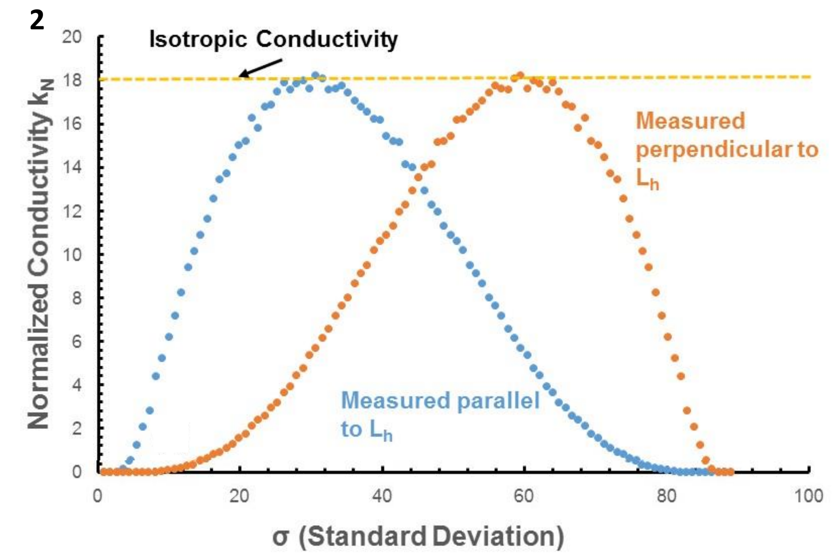
5) Results

1. Fix concentration of all samples at C_N = 29.1.
2. Increment width of distribution (20 trials/width).
3. Find conductivity parallel, perpendicular to alignment.

Hypothesis: *Directional increase in conductivity achievable in all configurations. Increase larger in more ordered configurations.*

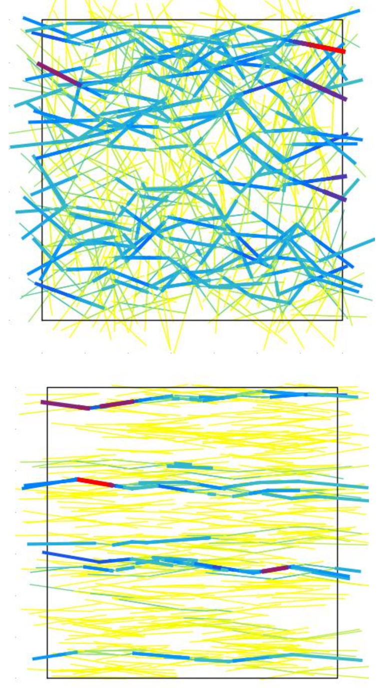


Normalized Conductivity vs σ, where orientation is restricted in range (-θ, θ)



Normalized Conductivity vs σ, where orientation is restricted in range [-θ] ∪ [θ]

- 1: Conductivity perpendicular to alignment decreases with orientation restriction.
- 1: Conductivity parallel to alignment optimized with slight orientation: ~**20% higher than isotropic conductivity.**
- Similar results for normal distribution.
- 2: Max conductivity (θ=30°) same as isotropic value.
- **Increase can be achieved through orientation, but highly ordered configurations are not ideal.**



- Results for 1 and 2 can be described as result of two competing effects. With increasing restriction:
  - Decrease in number of resistors (increases conductivity)
  - Decrease in amount of parallel paths (decreases conductivity)

Color/width shows amount of current. Top sample isotropic, right sample restricted orientation

6) Discussion and Conclusion

- Developed, verified model for conductivity of metal-NW networks.
- >20% increase in conductivity achievable w/ orientation. More ordered configurations not better.
- Advances foster displacement of ITO, pushing innovation in electronics.

Ongoing and Future Work

- Experimental orientation methods
- Adapt model to similar problems.
  - Traffic flow (ongoing)
- Test w/ R_J not dominant.
- Investigate nature of orientation effect more carefully (ongoing).

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