Network Analysis for Electrical Properties of Sheared Nano-Rod Dispersions

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Abstract

The first goal of this paper is to build a tight connection between two previously disjoint subjects: on one hand, complex networks, their graph representations, and graph analysis, and on the other hand, electrical properties of composite materials consisting of conducting rods or fibers dispersed in a poorly conducting matrix with at least one percolating path in the particle phase. This connection yields a new network analysis tool for experimental or numerical databases of a 3D rod or fiber dispersion. The novel application is for flow generated nano-rod and nano-fiber composites where particle number density overwhelms existing software and non-equilibrium, anisotropic distributions violate assumptions based on percolation threshold scaling behavior. The second goal of this paper is to apply this network analysis tool to the dimensional percolation phase diagram of sheared nano-rod dispersions [Zheng et. al. 2007]. The result is a statistical description of electrical properties appropriate to and consistent with statistical mechanics of nano-rod ensembles. The network analysis yields averaged conductance as well as local current and voltage distributions within the rod phase per realization.

1. Introduction

The properties of polymer nanocomposites have been extensively investigated during the past decades, but percolation-induced material properties of non-equilibrium oriented nano-rod systems are barely known. We focus on material systems with the following properties: the particles are highly conducting relative to the matrix; the rod or fiber orientational distribution is anisotropic, e.g., induced by a shear flow; and the particle phase has percolating clusters which span the physical sample. Our method consists of a series of steps.

- At a selected rod volume fraction (N) and normalized shear rate (Pe), generate the orientational PDF of a sheared nano-rod dispersion by the solution of the Doi-Hess-Smoluchowski equation [Forest et. al. 2004];
- Populate Monte Carlo samples of physical 3D sheared nano-rod dispersions by drawing from the PDF, decompose each MC realization into percolating cluster distributions;
- Map percolating cluster distributions to network graphs;
- Solve the graph electrical network problem, map back to MC samples, and generate statistics of properties and spatial geometry of load-carrying particles.

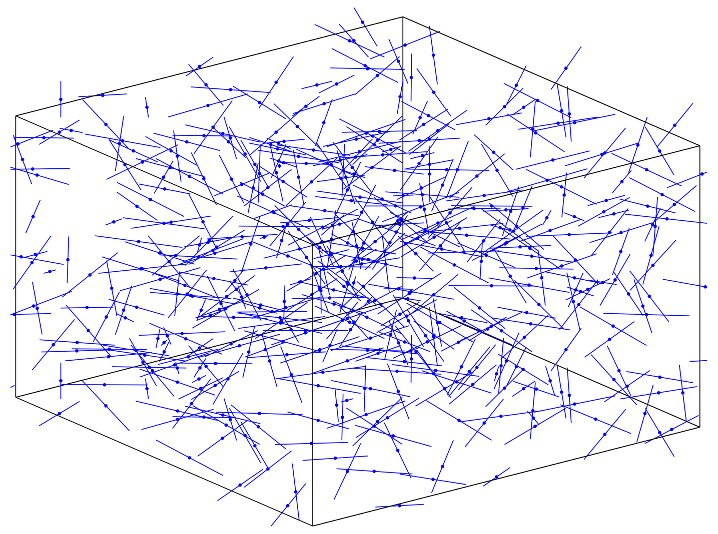
2. Model

2.1 Network Representation

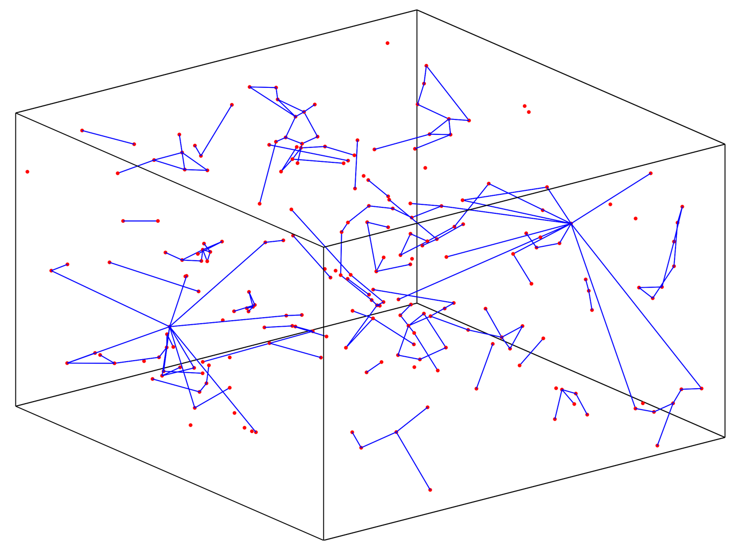
Nodes: Contact points of rods;

Edges: Effective resistance between contacts;

Two virtual nodes: Connections to external sources;



A randomly oriented dispersion, visualizing the individual rods.



Network representation of the electrical contacts between the rods, with two virtual nodes on opposing faces.

Adjacency matrix of the network:

$$\mathbf{A}_{ij} = \begin{cases} w_{ij} & \text{if node i and node j are connected} \\ 0 & \text{otherwise} \end{cases}$$

2.2 Electrical Properties

As described by Strang (1986), a linear system is constructed on the network:

$$\boldsymbol{L}\boldsymbol{v} = \boldsymbol{f}$$

where $\boldsymbol{v}$ is a vector consisting of the voltage at each vertex, $\boldsymbol{f}$ is a vector consisting of the net current going out of each node, and $\boldsymbol{L}$ is called the Laplacian matrix of the sub-network. $\boldsymbol{L}$ is related to the adjacency matrix $\boldsymbol{A}$ by $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$, with $\boldsymbol{D}$ being a diagonal matrix containing the degree of each node (i.e. sum of weights of all edges incident on the node). Kirchhoff's circuit law states that the net current going out of every node inside the network should be zero, so the voltage at each node inside the network results by solving equation given the voltage/current at the two virtual nodes. From the solution $\boldsymbol{v}$, the current distribution along edges in the network follows immediately, and the average conductance is computed as the ratio of the external current to the voltage drop between the two virtual nodes.

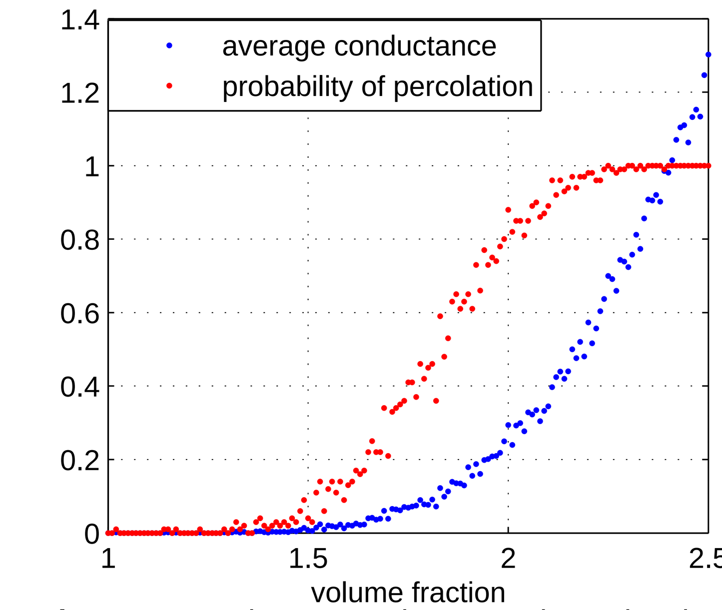
3. Simulation and Results

3.1 Simulation Procedures

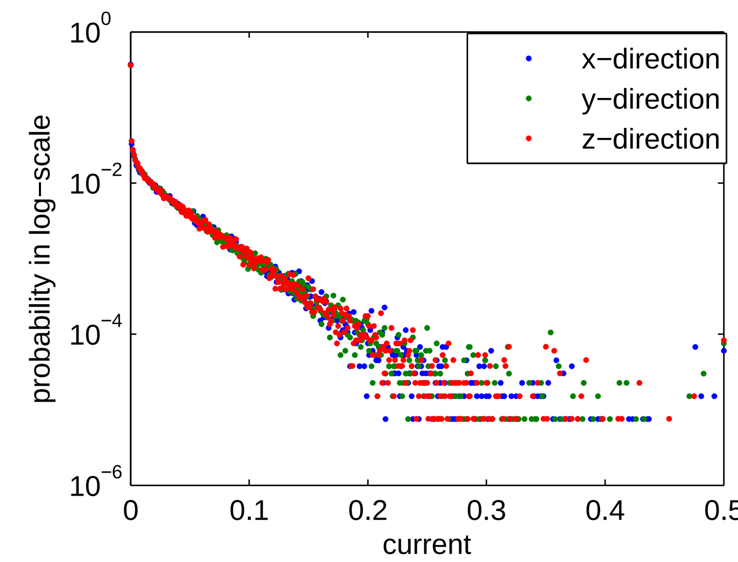
- Simulation is carried out across an (N,Pe) grid;
- At each parameter pair (N, Pe), firstly the orientational PDF is computed;
- Then 100 MC realizations are drawn from the PDF;
- Every sample is mapped to a graph and investigated using the network algorithm;
- Average over 100 samples and obtain a statistical description of electrical properties.

3.2 Numerical Results

For non-sheared (Pe=0) dispersions of aspect ratio 50

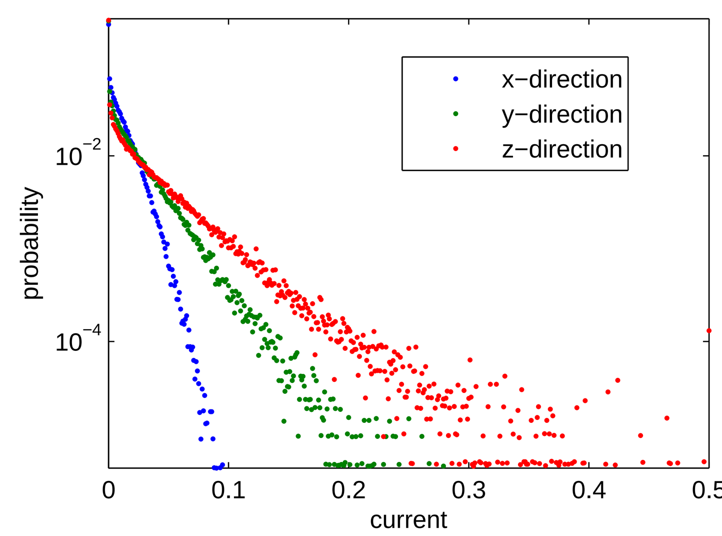


Average conductance along x axis and ratio of samples having percolating clusters along x axis for varying rod volume fraction

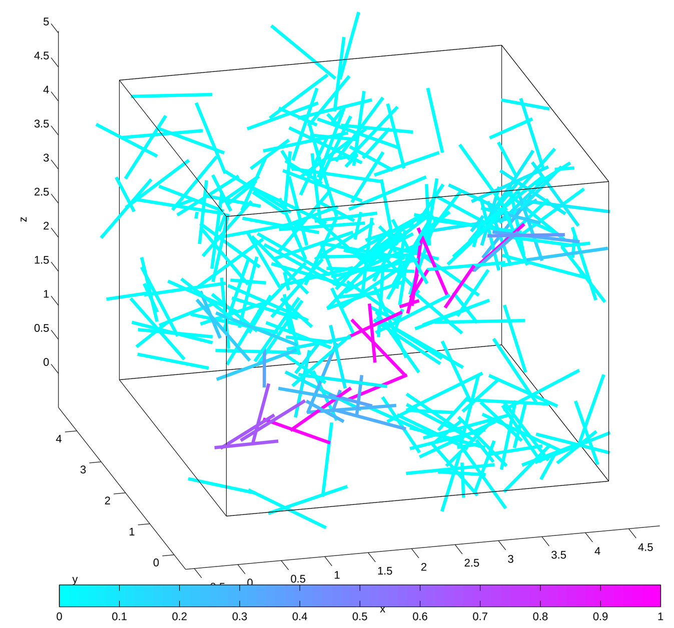


Current distributions in percolating clusters along x, y, z axes respectively for rod volume fraction 2.5%

For sheared dispersions of aspect ratio 50



Current distributions in percolating clusters along x, y, z axes respectively for rod volume fraction 2.5% and normalized shear rate 10



Visualization of current distribution along x axis for a single sample of rod volume fraction 1.9% and normalized shear rate 10

4. Conclusion

This paper addresses a theoretical and numerical gap in the electrical property characterization of nano-rod and nano-fiber composites, by introducing a network model of nanocomposite systems and utilizing network analysis tools. Our methods target the percolation-induced properties which dominate volume averaged properties and yield bulk electrical properties approaching those of the particle phase, for which there are limited results applicable to the onset of percolation thresholds.

References:
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