Percolation of Hard Rods in the Uniaxial Nematic Phase

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In geometric percolation, two hard particles are connected if their shortest surface-to-surface distance is smaller than some cut-off distance known as the connectedness criterion.[1] Clusters are then defined as collections of mutually connected particles. In a dispersion, the average number of particles in a cluster increases with increasing particle loading and diverges upon approach of the percolation threshold. The network of connected particles becomes system-spanning at the percolation threshold, and the physical properties of the dispersion change drastically beyond it. This is why the percolation threshold is an experimental observable.

For fluid dispersions of long rod-like particles, such as carbon nanotubes, the percolation threshold must depend on whether the particles are in the isotropic or in the uniaxial nematic phase, which for long rods appears at very low packing fractions. Theory and simulations have so far focused entirely on percolation in the isotropic phase. It is well-established now that for realistic connectedness criteria, percolation occurs near the isotropic-nematic phase transition,[2,3] and that alignment of the particles by external fields may shift or even suppresses it.[2,4]

We study percolation in the nematic phase of hard spherocylinders by means of Monte Carlo simulation and connectedness percolation theory. We find that there is a range of values of the connectedness criterion for which percolation does occur in the nematic phase, even under conditions where it does *not* occur in the isotropic phase. If the connectedness criterion drops below a critical value, then the percolation threshold shifts to concentrations in excess of that where the isotropic-to-nematic transition takes place.

We find that clusters of rod-like particles in the nematic phase are highly anisotropic, that is, they are very much longer along the director field than perpendicular to that. Still, upon approach of the percolation threshold both the length and the width of the clusters diverge with the same critical exponent. The fractal dimension of the clusters in the nematic phase remains two, the same value as of clusters in the isotropic phase, owing to the mean-field character of the theory.

The potential impact of twisted (cholesteric) order will be discussed.

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