Effect of dispersity of particle length on electrical conductivity of two-dimensional systems

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Abstract. By means of computer simulation, we examined the effect of dispersity of filler length on electrical conductivity of two-dimensional (2D) composites with rod-like fillers. A continuous approach was used. Highly conductive zero-width rod-like particles were deposited uniformly with given anisotropy onto a poorly conductive substrate. Length of particles varied according to the lognormal distribution. Our simulation evidenced that slightly disordered systems may have both high figure of merit, i.e., both high electrical conductivity and optical transmission simultaneously, and high electrical anisotropy.

1. Introduction
Transparent and flexible electrodes are important components of modern optoelectronic devices (see, e.g., [1] for review). Such electrodes are transparent, poorly conductive films containing highly conductive particles. Recently, simulations of electrical conductivity of two-dimensional (2D) composites with rod-like fillers have been performed both in lattice [2, 3, 4] and in continuous [5, 6] approaches. By contrast, fillers in real systems of conductive nanocomposites have different lengths following a lognormal distribution [7]. The goal of the present conference paper is to examine the effect of length dispersity on electrical conductivity of two-dimensional systems with rod-like fillers.

2. Methods
A continuous approach was used to prepare a 2D sample. Highly conductive zero-width rod-like particles were deposited uniformly with given anisotropy onto a poorly conductive substrate of size $L \times L$ subjected to periodic boundary conditions, i.e., onto a torus. The rods were allowed to intersect each other. The electrical conductivities of the particles and the substrate were $\sigma_p$ and $\sigma_m$, correspondingly. High electrical contrast $\Delta = \sigma_p / \sigma_m$ was assumed. Length of the particles, $l$, varied according to the lognormal distribution. We performed simulations for the fixed value of the mean length $\langle l \rangle = 1$ and different values of the standard deviation, SD = 0, 0.1, 0.5, 1.0.

The simulations were performed for different values of the order parameter defined as

$$s = N^{-1} \sum_{i=1}^{N} \cos 2\theta_i,$$  (1)

where $\theta_i$ is the angle between the particle and the substrate.
where $\theta_i$ is the angle between the axis of the $i$-th rod and the horizontal axis $x$, and $N$ is the total number of rods in the system. In our simulations, values of the order parameter were $s = 0, 0.5, 0.8, 1$.

To calculate the electrical conductivity of the film, the torus was unwrapped and transformed into a random resistor network (RRN) by means of discretization. A square mesh of $m \times m$ was applied to the film. When a cell of the mesh contained any part of a rod, it was assumed to be conductive and opaque. Otherwise, it was assumed to be insulating and transparent. The fraction of conductive (opaque) cells was denoted as $p$. The Frank–Lobb algorithm [8] was utilized to calculate the conductivity of the RRN. The percolation threshold, $p_c$, was found using the Hoshen–Kopelman algorithm [9].

A detailed description of our approach can be found in Ref. [10].

To characterize the electrical anisotropy, we used the quantity [2, 11]

$$\delta = \frac{\log_{10}(\sigma_\parallel/\sigma_\perp)}{\log_{10} \Delta},$$

(2)

where $\sigma_\parallel$ and $\sigma_\perp$ are the electrical conductivity along and perpendicular to the alignment of the fillers, respectively.

The figure of merit [12]

$$\Phi_{TC} = \frac{T^{10}}{R_s}$$

(3)

was calculated to characterize the films. Here, $T$ is the optical transmission and $R_s$ is the sheet resistance. In our computations, the optical transmission was taken as $T = 1 - p$. The sheet resistance $R_s$ was defined by

$$R_s = \frac{1}{\sigma t},$$

(4)

where $\sigma$ is the electrical conductivity and $t$ is the thickness of the film. Since the thickness of the film was constant in all our simulations, it was assumed to be 1 arbitrary unit in calculations of the figure of merit. Hence, the figure of merit was measured in arbitrary units.

To characterize the electrical properties of films at low concentrations of conductive rods, the “intrinsic conductivity”

$$[\sigma] = \left. \frac{d \ln \sigma}{dp} \right|_{p \to 0}$$

(5)

was calculated. This quantity was introduced [13, 14] by means the following virial expansion

$$\frac{\sigma}{\sigma_m} = 1 + [\sigma]p + O(p^2).$$

(6)

Throughout the text, the error bars in the figures correspond to the standard deviation of the means. When not shown explicitly, they are of the order of the marker size.

3. Results

Figure 1 demonstrates the effect of filler length dispersity on the figure of merit for two values of the order parameter. Both in the case of an isotropic system ($s = 0$) and in the case of a strictly anisotropic system, i.e., a system with completely aligned fillers ($s = 1$), an increase in the dispersity led to both an increase of the maximal value of the figure of merit and decrease of the number of fillers per area when this maximum occurred. Nevertheless, the figure of merit was significantly smaller (about 5 times) for the anisotropic system in compare with the isotropic case.

The results presented below were obtained for lattices with $L = 32$. Figure 2 shows, as an example, the results of a numerical calculation of the dependence of the logarithm of the
averaged effective electrical conductivity, $\sigma$, on the concentration, $p$, along the direction of alignment of the rods (a) and in the perpendicular direction (b) at SD = 0, 0.1, 0.5, 1.0 and $s = 0.5, m = 512$. The curves had the shape of a sigmoid; the jump in electrical conductivity indicated an insulator–metal transition. The concentration at which this transition occurred was reduced when the length dispersity increases in both perpendicular directions at partial ordering of the rods ($s = 0.5$). The number of long rods increases when the dispersity increased, which improved the connectivity of the system in both directions.

For an anisotropic system, the concentrations at which the transition occurred in perpendicular directions must be different, and figure 3 demonstrated this fact. Examples of the dependencies of the averaged effective electrical conductivity, $\sigma$, on the concentration, $p$, along the direction of alignment of the rods and in the perpendicular direction are presented in this figure at SD = 0.1, $s = 1, m = 1024$. The transition will occur at lower concentrations along the
alignment direction of the rods, since the appearance of long rods will affect the connectivity of the system primarily along the alignment direction.

Figure 3. Examples of the dependencies of the effective electrical conductivity, $\sigma$, on the concentration, $p$, SD = 0.1, $s = 1$, $m = 1024$, $L = 32$ along the direction of alignment of the rods (■) and in the perpendicular direction (●).

The more orderly the system was, the stronger this difference became (compare figure 4(a) for $s = 1$ and figure 4(b) for $s = 0.8$) at SD = 1, $s = 1$, $m = 1024$.

Figure 4. Examples of the dependencies of the effective electrical conductivity, $\sigma$, on the concentration, $p$, SD = 1, $s = 1$, $m = 1024$, $L = 32$ along the direction of alignment of the rods (■) and in the perpendicular direction (●): (a) $s = 1$; (b) $s = 0.8$.

The results obtained for the values of the percolation threshold, $p_c$, for different values of the length dispersity and the order parameter ($s = 0.5$, $0.8$, $1.0$) are summarized in figure 5. Here the value of the percolation threshold was normalized to ones at SD = 0, the results were given both for along the direction of alignment of the rods (closed symbols) and in the perpendicular direction (open symbols) and $m = 512$. The previously obtained conclusions were retained for all the investigated parameters $s$ and SD, except for the case when all the rods were aligned in one direction ($s = 1$) and the percolation threshold was determined in the direction perpendicular to the alignment direction. In this case, the value of the percolation threshold does not depend on the dispersity of the length of the rods, since the connectivity of the system in the direction perpendicular to the alignment did not depend on the length of the rods.

One of the important characteristics of the system is intrinsic conductivity; the results of its calculation are shown in figure 6. Here, the intrinsic conductivity along the direction of alignment of the rods, $[\sigma_\parallel]$, versus the aspect ratio of the rods, $k$, and the intrinsic conductivity
in the perpendicular direction, \([\sigma_\perp]\) versus \(1/k\) for the case of completely aligned rods \((s = 1)\) are given at \(SD = 0, 0.1, 0.5, 1\). The aspect ratio was calculated as \(m/L\) for three values \(m = 256, 512, 1024\). The lines are a linear approximation.

**Figure 5.** Examples of the normalized percolation threshold, \(p_c/p_{c0}\), versus \(SD\) for three values of the standard deviation \(SD\) at \(s = 0.5\) (□, ■), 0.8 (○, ●), 1.0 (△, ▲) (closed and open symbols correspond to the direction along alignment of the rods and in the perpendicular direction, correspondingly) and \(m = 256\). Here, \(p_{c0}\) corresponds to \(SD = 0\).

**Figure 6.** The intrinsic conductivity along the direction of alignment of the rods, \([\sigma_\parallel]\), vs the aspect ratio, \(k\), of the rods (closed symbols, solid lines) and the intrinsic conductivity in the perpendicular direction, \([\sigma_\perp]\) vs \(1/k\) (open symbols, dotted lines) at \(SD = 0\) (□, ■), 0.1 (○, ●), 0.5 (△, ▲), 1 (▽, ▼) for the case of completely aligned rods \((s = 1)\).

**Figure 7.** Example of the dependencies of the electrical anisotropy ratio, \(\delta\), versus the concentration, \(p\), for \(SD = 0.1, 0.5, 1\), \(m = 512\): (a) \(s = 1\), (b) \(s = 0.8\). In the case \(s = 0.8\), partial arrangement of the rods (figure 7(b)), the maximum of the electrical anisotropy ratio was shifted to the region of smaller values \(p\) and the interval of \(p\) for large electrical anisotropy was smaller compared with completely aligned fillers \((s = 1)\) (figure 7(a)).

**Figure 7.** Example of the dependencies of the electrical anisotropy ratio, \(\delta\), vs the concentration, \(p\), for different values of the length dispersity \(SD = 0.1\) — — — — , 0.5- - - - , 1——, \(m = 512\) and \(L = 32\): (a) completely aligned rods \(s = 1\); (b) \(s = 0.8\).
4. Conclusion
Our computer simulation suggests that the dispersity of the filler length had a significant impact only at the electrical conductivity of films along the direction of the filler alignment; the electrical conductivity in the direction perpendicular to the filler alignment was insensitive to the dispersity of the filler length. This dispersity had a positive impact on the figure of merit of films. It decreased the percolation threshold and, as a result, the critical concentration of fillers when the insulator–conductor phase transition occurred. In the vicinity of the phase transition, the electrical conductivity of the film exhibited high anisotropy.

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