

Efficient resistor network simulation method for graphene-based conductor materials

Leo Rizzi^{1,3}

Andreas Zienert¹, Jörg Schuster², Martin Köhne³, Stefan E. Schulz^{1,2}

¹ETIT, TU Chemnitz, Str. der Nationen 62, 09111 Chemnitz, Germany

²Fraunhofer ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany

³Robert Bosch GmbH, Robert-Bosch-Campus 1, 71272 Renningen, Germany

leo.rizzi@s2017.tu-chemnitz.de

In recent years, graphene fibers (GFs) have emerged as a new form of electrical conductors in an effort to transfer graphene's extraordinary properties to the macroscopic scale [1]. They consist of an assembly of graphene sheets spun into a textile fiber. GFs are lightweight, mechanically strong, and corrosion resistant. Defect-engineering and doping strategies have continuously improved the electrical conductivity of fibers towards metallic levels [2]. However, the conductivity of GFs still remains below the conductivities of silver or copper.

While several groups have presented experimental results on the production of GFs, theoretical descriptions predicting their electrical behavior are less advanced. In order to identify the key parameters for an optimum conductivity of GFs, we present an efficient simulation method. The electrical conductivity of GFs is modelled by means of a three-dimensional random network of resistors (Fig. 1). We investigate the influence of various material properties such as graphene sheet conductivity (Fig. 2), size distribution, or packing density on the fiber electrical conductivity. We compare our results to an analytical network model which reproduces relevant features despite its simplicity.

Our findings offer a deeper understanding of GFs and can be helpful to further enhance their electrical performance. Furthermore, the method can be transferred to any bulk-like material that is composed of two-dimensional building blocks.

References

- [1] Zhen Xu, Chao Gao, Nature Communications, 2 (2011) 571
- [2] Yingjun Liu, Zhen Xu, Jianming Zhan, Peigang Li, Chao Gao, Advanced Materials, 36 (2016), 7941

Figures

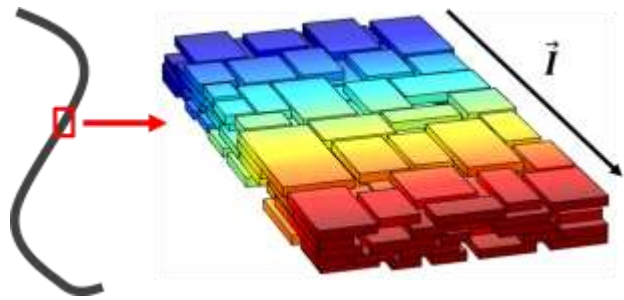


Figure 1: Graphene fiber model based on a random graphene flake distribution

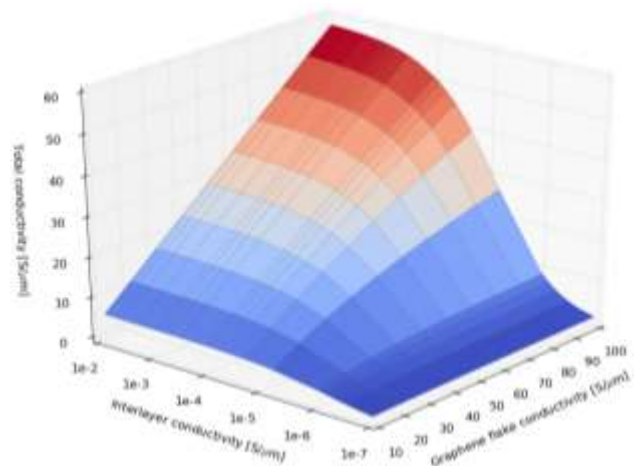


Figure 2: Graphene fiber parameter study. Total conductivity as a function of intralayer and flake conductivity.