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Effect of the grain boundaries on the electronic and mechanical structure of graphene

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The grain boundaries in the graphene nanostructures usually consist of a combination of pentagonal and heptagonal defects. Being not very thick, they create regions of size tenths of nanometers. They arise during the production process and are intimately connected with the internal structure of the corresponding materials. The production process is mostly initiated by the chemical vapor deposition. Of course, the grain boundaries have a huge, usually undesirable influence on the electronic structure of the materials. Depending on the external conditions during the production, there can be qualitative differences in their properties. The resulting structures contain grains of different sizes, distributions and lattice orientations. Numerical calculations for a few samples were performed where the average sizes of the grains fluctuated from 13 to 25nm. They showed a considerable difference in the conductivities and charge carrier mobilities. The mobilities depend on the size of the grain boundaries linearly. Next, different configurations of the defects in the grain boundaries were considered and the corresponding polycrystalline structures showed significant differences in the investigated characteristics.

Biography

Jan Smotlacha has completed his PhD at the age of 33 years from Czech Technical University. Now he works as the senior research scientist in the Bogoliubov Laboratory of Theoretical Physics in the Joint Institute for Nuclear Research in Dubna. His investigation is concentrated on the graphene and other kinds of nanostructures and Weyl semimetals. Besides the electronic and magnetic properties, he models the influence of the structure perturbations connected with the topological defects and geometry. He has published about 20 papers in reputed journals or conference proceedings.

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