Polycrystalline graphene: atomic structure and electronic transport properties

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Abstract There is growing evidence of the polycrystalline nature of graphene samples at micrometer length scales [1-3]. Grain boundaries and dislocations, intrinsic topological defects of polycrystalline materials, inevitably affect all kinds of physical properties of graphene. This talk reviews our theoretical efforts directed towards understanding the atomic structure and electronic transport properties of polycrystalline graphene. Recent experimental works on this subject are also covered in the presentation.

In the first part of my talk, I will introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors and grain boundaries covering the complete range of possible misorientation angles [4]. By means of first-principles calculations we address the thermodynamic properties of grain boundaries revealing energetically favorable large-angle configurations as well as dramatic stabilization of small-angle configurations via the out-of-plane deformation, a remarkable feature of graphene as a two-dimensional material.

The rest of my talk will cover on the electronic transport properties of polycrystalline graphene focusing on the following two scenarios. Ballistic charge-carrier transmission across the periodic grain boundaries is shown to be governed primarily by a simple momentum conservation law [5]. Two distinct transport behaviors are predicted − either perfect reflection or high transparency with respect to low-energy charge carriers depending on the grain boundary periodicity. Beyond the momentum conservation picture we find that the transmission of low-energy charge carriers can be dramatically suppressed in the small-angle limit. This counter-intuitive behavior is explained from the standpoint of resonant backscattering involving localized electronic states of topological origin [6].

These results demonstrate that dislocations and grain boundaries are intrinsic topological defects which dramatically affect the transport properties of graphene and can also be used for engineering novel functional devices [7].

References

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