Polycrystalline graphene: atomic structure and electronic transport properties

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There is growing evidence of the polycrystalline nature of graphene samples at micrometer length scales. 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 atomic structure and electronic transport properties of polycrystalline graphene. Recent experimental works on this subject are also covered in my lecture.

We introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors and grain boundaries covering the whole range of possible misorientation angles [1]. By using ab initio calculations we investigate thermodynamic properties of grain boundaries finding energetically favorable large-angle symmetric configurations as well as dramatic stabilization of small-angle configurations via the out-of-plane deformation, a remarkable feature of graphene as a truly two-dimensional material. Charge-carrier transport across periodic grain boundaries in graphene is shown to be governed primarily by a simple momentum conservation law [2]. Two distinct transport behaviors are predicted - either perfect reflection or high transparency for low-energy charge carriers depending on the grain boundary structure. Beyond the momentum conservation picture we find that the transmission of low-energy charge carriers can be dramatically suppressed in the sma ll-angle limit [3]. This counter-intuitive behavior is explained from the standpoint of resonant backscattering involving electronic states localized at the dislocations. Finally, my talk will cover advances of a joint experiment-theory project on controlled engineering of a degenerate grain boundary defect exhibiting valley-filtering properties [4].

These results demonstrate that dislocations and grain boundaries are important intrinsic defects in graphene which can be used for engineering novel functional devices.

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