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Defect Dynamics in Graphene

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ABSTRACT

The experimental and theoretical study of graphene, two-dimensional (2D) graphite, is an extremely rapidly growing field of today's condensed matter research. Different types of disorder in graphene modify the Dirac equation leading to unusual spectroscopic and transport properties. The authors studied one of the disorders (i.e., grain boundaries) and formulated a theoretical model of graphene grain boundary by generalizing the two-dimensional graphene Dirac Hamiltonian model. In this model only, the authors considered the long-wavelength limit of the particle transport, which provides the main contribution to the graphene conductance. In this work, they derived the Hamiltonian in a rotated side dependent reference frame describing crystallographic axes mismatching at a grain boundary junction and showed that properties like energy spectrum are an independent reference frame. Also, they showed one of the topological property of graphene.

KEYWORDS

Dirac Equation, Disorders, Grain Boundaries, Graphene

1 INTRODUCTION

It is the second law of thermodynamics that dictates the presence of a certain amount of disorder in crystalline materials. But it is also due to the imperfection of material production processes that impurities and defects are always present in crystals. Such lattice imperfections have a strong influence on the electronic, optical, thermal, and mechanical properties of the solid. In fact, many of the characteristics of technologically important materials such as the conductance of semiconductors or the mechanical strength and ductility of metals are governed by defect (Kittel, 1953).Defects in bulk crystals have been studied extensively for many decades. Two dimensional crystals, however, have been considered only recently. Two graphite rods from two empty mosquito repellent refills were employed for synthesis of few-layered graphene for material developments on batteries and

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supercapacitor applications. The graphene sheet is isolated from graphite rod via electrochemical exfoliation method (Udhaya Sankar, 2018).

In fact, it was believed for a long time that they would be structurally unstable because of long wavelength fluctuations according to the Mermin Wagner theorem (Mermin, 1968). The situation changed, however, when single-layers of graphene were isolated for the first time by mechanical exfoliation (Novoselov, 2004). Graphene consists of a hexagonal monolayer network of sp2 - hybridized carbon atoms. Graphene and its structural counterpart, hexagonal boron nitride, are the only two-dimensional crystalline materials we know today (Geim, 2009) (Britnell, 2012). The properties of graphene were expected to be outstanding, based on calculations addressing graphene as the parent material for carbon nanotubes. Therefore, the availability of graphene for experiments initiated a massive body of research, especially after large-scale synthesis methods like chemical vapor-deposition (Bae, 2010) and epitaxial growth (Kim, 2009) (Berger, 2004) on metal and SiC substrates were developed. Indeed, the predicted extraordinary properties have now been confirmed in many studies. Graphene is a single layer of graphite, the remarkable about it is that its crystalline structure is two dimensional. In other words the atoms in graphene are laid flat like billiard balls on a table. Just like in graphite each layer of graphene is made of hexagonal rings of carbon like lots of benzene rings connected together only with more carbon atoms replacing hydrogen atoms around the edge giving graphene a honeycomb structure. Some of these properties can only be observed at an extremely low defect concentration, which, as we discuss later, is possible because of the high formation energies of point defects in graphene. Nevertheless, like in any other real material, structural defects do exist in graphene and can dramatically alter its properties. Defects can also be deliberately introduced into this material, for example, by irradiation or chemical treatments which change graphene from crystalline to amporphous.

Graphene is a two-dimensional honeycomb lattice constituted by carbon atoms (Shah M. A and Shah K.A). Its reciprocal lattice determines a hexagonal Brillouin zone having six corners (K/K' points) where the low energy part of the bands structure is well described by a linear energy-momentum dispersion relation, defining the so-called Dirac cone. The existence of Dirac cones in the graphene bands structure can be understood by using a tight-binding model. Consequently, the particle dynamics in graphene lattice follows the Dirac equation (Sarma, 2011), being the latter the manifestation of an emergent ultra relativistic behavior in a many-body system initially described by the Schr¨odinger equation. Due to its unique band structure, in the past few years graphene has attracted much attention and intriguing transport properties, such as Klein tunneling (Allain, 2011), Zitterbewegung effect (Rusin, 2008), antilocalization (Tikhonenko, 2009), anomalous quantum Hall effect (Ostrovsky, 2008), Veselago focusing effect (Cheianov, 2007), have been suggested and, in some cases, experimentally proven. Apart from its theoretical interest, graphene is a two-dimensional chemical homogeneous system characterized by very high electrical mobility (Banszerus, 2015) and extraordinary mechanical properties (Papageorgiou, 2017), making it appealing in nanoelectronics and for flexible electronics implementations(Lee, 2015).

Crystals are never perfect and have various types of imperfections. These defects may affect many of their physical and mechanical properties, which in turn affect many important engineering properties. Graphene has been attracted a lot of interests as one of fashionable materials since it has opened horizons for physics exploration and future technology as a two dimensional material with extraordinary physical properties (Novoselov K. S., 2005) (Geim A. K., 2010). In general, the properties of graphene can be affected by structural irregularities such as dislocation, grain boundary, and edge structure (Han, 2007) (Son, 2006) so that those defect structures in graphene have been subjects of study. These imperfections are classified according to their geometry and shape. Of them the two dimensional defects that include external surfaces and grain boundaries have profound effect on electronic states of materials. The properties of polycrystalline materials are often dominated by the size of their grains and by the atomic structure of their grain boundaries. These effects should be especially pronounced in two dimensional materials, where even a line defect can divide and disrupt