Author's Accepted Manuscript

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PII: S0022-5096(14)00092-1
DOI: http://dx.doi.org/10.1016/j.jmps.2014.05.009
Reference: MPS2478

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 7 January 2014
Revised date: 14 April 2014
Accepted date: 12 May 2014

Cite this article as: Zhuhua Zhang, Yang Yang, Boris I. Yakobson, Grain boundaries in Hybrid two-dimensional materials, *Journal of the Mechanics and Physics of Solids,* http://dx.doi.org/10.1016/j.jmps.2014.05.009

Grain boundaries in hybrid two-dimensional materials

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In two-dimensional (2D) materials, bisector grain boundaries (GBs) are energetically favorable as they allow perfect match of neighbor grains. We demonstrate here a contrasting behavior for GBs in hybrid 2D materials, which tend to be non-bisector and obey a universal law to optimally match the heterogeneous grains: the ratio of cosines of the rotation angles of two neighbor grains equals the ratio of constituent's lattice parameters, reminiscent of Snell's law for light refraction. Details of the optimal GB structures are further formulated in terms of tilt angle, lattice mismatch strain and deviation angle from the bisector line, in good agreement with comprehensive numerical analyses. The ground state structures of the GBs manifest as a series of laterally misaligned bisector segments, which are verified by intensive first-principles calculations. Our findings not only provide a general guidance for exploring GBs in various hybrid 2D materials but also serve as an important stepping stone for understanding mechanical and electronic behaviors in these 2D nanoscale patchworks.

Keywords: grain boundary, two dimensional material, hybrid material, dislocations, first-principles calculations

1. Introduction

In the past few years, two-dimensional (2D) materials have undergone a flurry of research activities, leading the science and technology for low-dimensional materials into a 2D age. Among various 2D materials synthesized thus far, graphene(Novoselov et al., 2005) and single-layered hexagonal boron nitride (h-BN) (Zhang et al., 2005; Geim and Novoselov, 2007; Castro Neto et al., 2009) have attracted particular research attention, not only owing to similar hexagonal honeycomb lattices but also because of their supreme mechanical properties (Lee et al., 2008; Chang and Gao, 2003; Chang et al., 2006). However, graphene is a zero-gap semi-metal, while the h-BN monolayer is electrically insulating with a wide band gap ~5.8 eV (Nag et al., 2010; Golberg et al., 2010; Zhang and Guo, 2008; Jin et al., 2009; Jiang and Guo, 2011). The distinct properties of the two hexagonal isologues have stimulated great interests in fabricating hybridized atomic layers composed of graphene and BN domains—a new 2D BNC material with properties complementary to those of its constituents (Ci et al., 2010; Sutter et al.,2012; Liu et al., 2013; Gao et al., 2013; Liu, et al., 2011). Of most interest is that varying the ratio of composition could endow the hybrid BNC sheet with tunable band gap on-demand, ranging from 0 eV to 5.8 eV (da Rocha Martins et al., 2010; Ramasubramaniam and Naveh, 2011; Bhowmick et al., 2011; Jung et al., 2012; Muchharla et al., 2013; Ding et al., 2009; Lu et al., 2010). Moreover, having BN domains patched in otherwise perfect graphene structures leads to