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ScienceDirect

Procedia IUTAM 21 (2017) 17 – 24

Procedia IUTAM

www.elsevier.com/locate/procedia

2016 IUTAM Symposium on Nanoscale Physical Mechanics

Mechanics of materials creation: nanotubes, graphene, carbyne, borophenes

John M. Alred, Nitant Gupta, Mingjie Liu, Zhuhua Zhang, Boris I. Yakobson*

Department of Material Sicnece and NanoEngineering, Rice University, 6100 Main St, Houston, TX 77005, USA

Abstract

In this article, we provide brief overview of how mechanics and computations play a role in understanding materials growth, creating new low-dimensional materials and exploring structural defects. First, we introduce a concept of screw dislocation for describing carbon nanotube growth and derive a kinetic relationship between growth rate and chiral angle. Deeper analysis of the subtle balance between the kinetic and thermodynamic views reveals sharply peaked distribution of near-armchair nanotubes, explaining puzzling (n, n-1) types observed experimentally. A combination of *ab initio* calculations and Monte Carlo models further explains the low symmetry shapes of graphene on substrates. Being monoatomic chains of carbon, carbynes are shown to be strong yet flexible, and undergo metal-semiconductor transition under tension, offering promising innovations for future nanotechnology. We then reveal how metal substrates could facilitate the formation of boron monolayers whose bulk counterparts are non-layered and lower in energy. Further remarks are given to High Burger's vector graphene defects called D-loops and interfaces in hybrid graphene-BN materials, both with significant out-of plane distortion and impact on the mechanical properties. All of these computationally modeled systems have significant implications for the future use of these nanomaterials.

Keywords: mechanics, low-dimensional, graphene, carbyne, boron

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* Corresponding author. Tel.: +1-713-348-3572.
E-mail address: biy@rice.edu

doi:10.1016/j.piutam.2017.03.032

1. Introduction

Mechanics of materials is often about the deformations and ultimately failure. We will discuss how the concepts of mechanics bear fruit in unusual field of synthesis, when material structure is created through the self-assembly of constituent units, atoms. A recent cover article in C&EN offers a broad retrospect of carbon nanotube research within a framework of Gartner's hype peak [1], tacitly inviting the readers to similarly gauge the peak phases for graphene, or materials "beyond" graphene, say carbyne, transition metal dichalcogenide monolayers, h-BN, or pure boron. We will give several examples of works in our research group, where equations and computers are used to understand and predict materials, including carbon nanotubes, graphene, carbyne and borophenes. Further remark will be given to some novel defects and interface structures predicted in carbon materials and as well as the exotic mechanical properties these defects bring out.

2. Carbon nanotube and graphene

The growth mechanism of carbon nanotubes (CNTs) and graphene has been a critical issue to realizing their controlled synthesis, which has been of great challenge for over two decades. The CNTs have a perfect cylindrical geometry that is periodic along the tube axis, suggesting that their growth should obey basic rules established for normal crystals. Inspired by the concepts established for macroscopic crystals, we introduce an axial screw dislocation for describing the CNTs, whose chiral angle can be distinguished by the magnitude of the Burgers vector of such dislocation. A kinetic analysis, combined with first-principles calculations, revealed that growth rate of CNTs is proportional to the Burgers vector and therefore the chiral angle[2], resulting in a kinetic formula $R \sim \sin x$, where R is growth rate and x is the chiral angle. This formula is in excellent agreement with experiments[3].

During the process of synthesis, the growing CNT needs to contact with a solid catalyst (usually transition metal clusters), which introduces additional binding energy between the tube and catalyst. The armchair and zigzag CNTs would have tight contact with the catalyst but suffer from low growth rate as the atomic accretion is difficult due to a small space between the tube and catalyst. One the other hand, the CNT with a large chiral angle favors the attachment of carbon atoms for maintaining the growth but has a unfavorable loose contact with the catalyst. Detailed analysis of the subtle balance between the kinetic and thermodynamic views reveals sharply peaked abundance distribution of CNT chirality $A \sim x \exp(-x)$ [4]. This equation well explains the puzzling $(n, n\text{-}1)$ types observed in many experiments[5,6].

The graphene growth is highly similar to CNTs, in a sense that they both need metal catalysts and their contacts with catalysts govern the growth process. Building on our above approach, we further combine density functional theory method and Monte Carlo models to explore the symmetry effect of metal substrates on the graphene growth. The stacking registry between graphene and substrate, and growth kinetics in which the carbon attaches to the edge atom by atom are shown to determine the shape of graphene islands[7]. In particular, the substrate-induced variations of edge energy δE can only result in distorted hexagons for the thermodynamic equilibrium shape as the shape linearly depends on δE; whereas δE enters the growth rate exponentially as $R \sim e^{\delta E/k\mathrm{BT}}$, which significantly amplifies the symmetry breaking. As a result, the shape is completely changed to the frequently observed triangular and even lower symmetry shapes of graphene synthesized on metals[8,9].

3. Carbyne

The rich bonding types of carbon enables it to form a structure with even lower dimensionality—one dimensional carbon atomic chain, named as carbyne. It is one of the allotropes of carbon with purely *sp* hybridization. It was proposed theoretically that carbyne may be stable at high temperature.[10] In recent years, there are a number of experimental reports on fabricating finite-long carbon chains. Many interesting applications of carbynes have also been proposed theoretically, including nanoelectronic/spintronic devices,[11–14] and hydrogen storage.[15] One of the impressive properties is its mechanical property.[16] Starting from the structure, there are two structures of this linear atomic carbon chain: one is cumulene (=C=C=) with equal bond length; the cumulene structure undergoes a Peierls transition to dimerize into the polyyne (–C≡C–) structure (Figure 1, left). The polyyne structure is favoured by 2 meV per atom over cumulene according to density functional theory calculations. The mechanical properties