doi:10.1017/S1431927610058897
Microsc. Microanal. 16 (Suppl 2), 2010

Ultra-High-Resolution Transmission Electron Microscopy of Atomically Thin Hexagonal Boron Nitride (h-BN)

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Atomically thin 2D ordered crystals, such as graphene and hexagonal boron nitride (h-BN), are considered new emerging materials with potential applications in sensing and in the electronic industry [1-5]. The electrical, thermal, chemical and mechanical properties of such crystals are strongly influenced by their atomic structure. Therefore, understanding the atomic scale stability and dynamics of defects and vacancies with the add-atoms and molecules in such membrane systems is crucial to predict their resulting properties and potential applications. While graphene is a zero band gap material with high carrier mobility, h-BN is a wide band gap insulating material with potential applications in hydrogen storage and DUV light emitters [1, 3]. Graphene and h-BN both consist of single sheets of sp^2-bonded atoms forming a honeycomb cell structure [6-7]. They, however, have different atomic stackings. In h-BN the boron atoms are stacked on top of nitrogen on the adjacent planes resulting in AAA atomic layer stacking, while graphite forms a Bernal Stacking sequence.

In a recent study, we have successfully isolated one monolayer (1 ML) of h-BN and have unambiguously identified the boron atom from nitrogen in a unit cell of an atomically thin h-BN using an ultra-high-resolution transmission electron microscope [8]. Figure 1a shows a high resolution TEM image of h-BN taken by the TEAM 0.5 microscope located at the National Center for Electron Microscopy (NCEM). This image shows a one- to four-layer region of h-BN with vacancies and holes. Using high resolution TEM imaging, we use the projected potential of the atoms to unambiguously identify their chemical nature (boron or nitrogen) throughout the sample. To enhance the signal to noise ratio in this identification, we consider the projected potential of the summation of twenty unit cells in h-BN for each layer thickness. According to the intensity line profile of the h-BN unit cell, a clear asymmetry is observed in the projected potential of the atoms in the adjacent h-BN columns in the odd layer-number regions (n=1 and 3). No discernible asymmetry, however, is observed for adjacent columns in even-layer-number regions (n=2 and 4). Figure 1b shows the nitrogen atom yielding the stronger intensity in the unit cell images with 1 and 3 ML. This atom identification technique has further enabled us to study the nature of defects and edges in h-BN. We observe that defects in h-BN are formed mainly as a result of the ejection of boron atoms from the lattice, while the edges are in the form of nitrogen-terminating zigzag edges.

Single layer 2D crystal membranes offer a unique model system to study the stability and dynamics of defects, edges and vacancies, and their interactions with adatoms or molecules. In this investigation, we address the stability and dynamics of vacancy formation in h-BN and the interaction dynamics between the adatoms/molecules and the defects/edges in this membrane.

Figure 2 presents consecutive images of a double-layer of h-BN indicating the formation and migration of vacancies and their interaction with the molecules.

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[9] This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the US Department of Energy under Contract DE-AC02-05CH11231, and detailed TEAM 0.5 characterization at the NCEM.

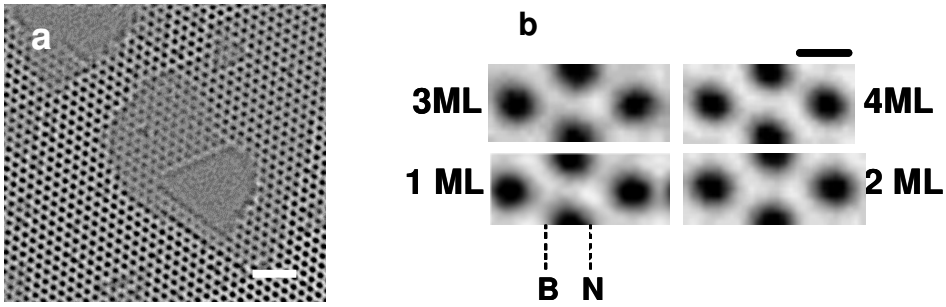

FIG. 1. (a) Reconstructed TEM phase image of h-BN (scale bar is 1 nm). (b) The resulting images from the summation of 20 unit cell images in a one- to four-layer BN. The scale bar shows 1.5 Å.

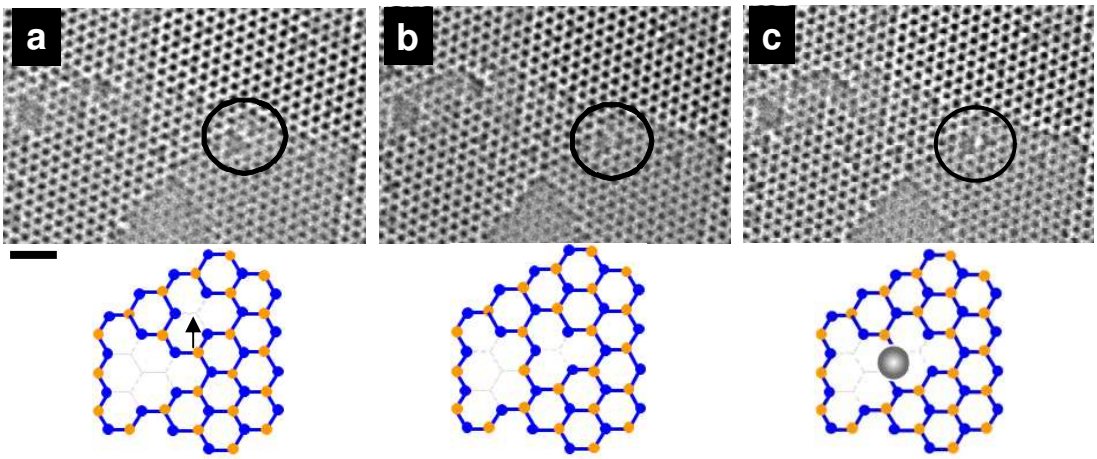

FIG. 2. Marked within the circle is a double-layer of h-BN showing the stability and dynamics of vacancy formation and its interaction with a light molecule. (a) A large triangular vacancy formed after ejection of three boron and one nitrogen atoms. Also shown is a boron mono-vacancy at the edge of the large vacancy. (b) Within two seconds, the boron mono-vacancy migrates after diffusion of the edge-boron atom (shown by an arrow on Fig. 2a) resulting in a new vacancy arrangement. (c) A molecule was absorbed on top of the zigzag vacancy edge after a couple of seconds. In this representation boron atom is orange and nitrogen is blue. (scale bar is 1 nm)

https://doi.org/10.1017/S1431927610058897 Published online by Cambridge University Press