Simulating Boron Nitride Nanostructure Interactions

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ABSTRACT

Boron nitride (BN) nanostructures have long been regarded as one of the most promising inorganic nanosystems due to their stiffness, thermal conductivity, and stability. These structures have been successfully and efficiently synthesized using plasma arc discharge. Although the structure of these nanosystems have long been studied, the process through which they form is still not completely understood. Using the latest version of the DFTB+ (Density Functional based Tight Binding) code, we were able to study the interaction between hydrogen and BN nanotubules and the effects of hydrogen on BN nanostructure synthesis and growth.

BACKGROUND

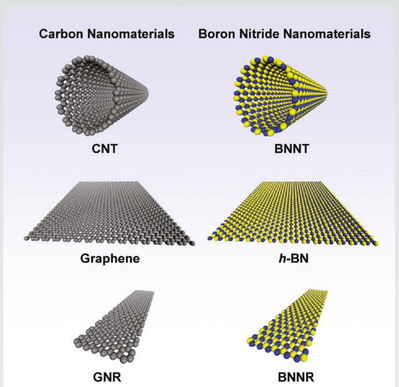


Figure 1. A depiction of the structural similarities between carbon and BN nanostructures.

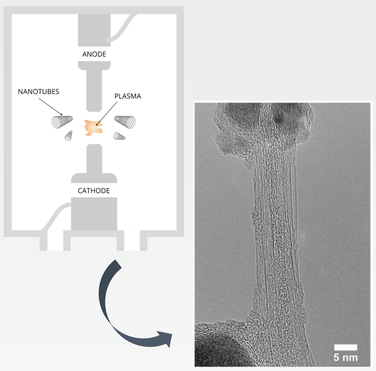


Figure 2. (left) The plasma arc synthesis method consists of the following: an inert gas environment, the anode which holds the material to be ablated, and the cathode on which the nanostructures are formed.
Figure 3. (right) Example of a single-walled BNNT cluster formed in plasma arc.[3]

Boron nitride is a compound of boron and nitrogen with the chemical formula BN.

- Great thermal stability and resistant to oxidation
- Exists in various crystalline forms that are isoelectronic to structures seen in carbon: amorphous (a-BN), hexagonal (h-BN), cubic (c-BN), and the rare wurtzite (w-BN)
- BN nanotubules (BNNTs) are particularly useful and they hold similar structure to that of carbon nanotubules (see Figure 1)

Plasma arc discharge method for growing BNNTs

- A physical method of *nanosynthesis* uses a plasma arc to vaporize/ablate material
- Plasma is achieved by making a gas conduct electricity when a potential difference (DC) is applied between two electrodes (see Figure 2)
- *Arc discharge* – the electrical breakdown of gas which results in an ongoing plasma discharge

Nanotubes are formed from h-BN sheets (BN flakes) that roll onto themselves

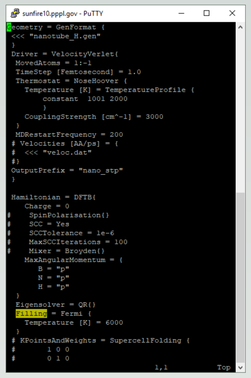
- BNNTs were predicted in 1994 and experimentally discovered in 1995[1]
- Defined as cylinders with sub-micrometer diameters and micrometer lengths (high aspect ratio), with rings formed of alternating boron and nitrogen atoms.
- One of the strongest, light-weight nanomaterials with a Young's modulus of > 1 TPa and possesses a much wider band gap than CNTs (~5.5 eV)[2]

OBJECTIVES

- Install and compile DFTB+ with MPI on the PPPL and NERSC clusters
- Study the development of BN structures on a boron liquid droplet
- Study the interactions of hydrogen with BNNTs and design simulation
- Write a basic guide on the usage of DFTB+ and Jmol for the simulation of nanostructures

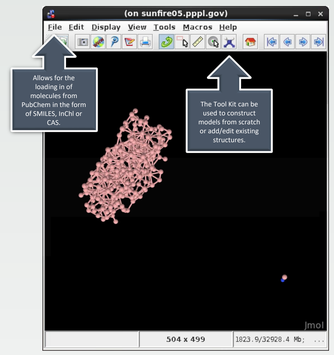
METHODS

- DFTB+ is a versatile quantum mechanical simulation software package. It is based on the Density Functional Tight Binding (DFTB) method and can carry out quantum mechanical simulations similar to DFT but in an approximate way.
  - Can run approximately twice as fast[4] as other simulation methods.
- Density Functional Theory (DFT) is a method of approximating QM solutions for multiple electron systems.
  - Computationally less intensive than ab-initio and semi-empirical methods.
  - Adequate for calculating structures and energies for medium-sized systems.
  - Difficulty describing Van der Waals forces and in calculating band gap
- The Tight Binding model or (TB) is an approach to the calculation of electronic band structure (including band gap).
  - Uses an approximate set of wave functions from superimposed wave functions for isolated atoms at each atomic site.
  - Electrons in this model should be tightly bound to atom, usually solid-state.
  - Can be combined with other models to improve approximations.
- Structures and simulations
  - Structures were either grown by starting with input file provided by Longtao Han or created from scratch using Jmol application.
  - Program written in C was used to create an environment in which a given structure was bombarded by the user's choice of atom(s).
- Jmol is an open-source viewer for three dimensional models.
  - Program was used to create structures and view time-steps of each simulation.



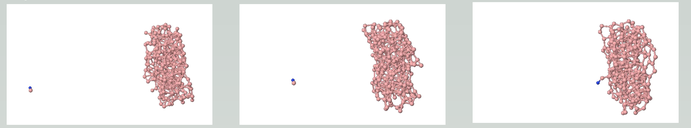
An example of the input file used for DFTB+ simulations. The program is able to read either Human-readable Structured Data (HSD) or XML. The different blocks specify the various properties of the simulation, such as the boundary conditions, if and how the geometry of the structure will change,

Deciding upon the model used is easy, given that DFTB+ currently only supports Density Functional based Tight Binding Hamiltonians.

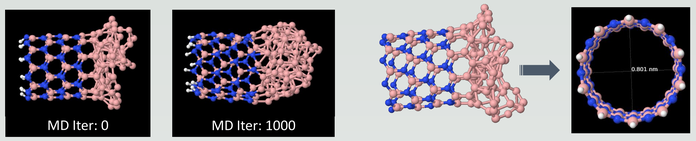


RESULTS

- First successful simulation depicted a large boron liquid droplet being bombarded by BN molecules.



- Run over the course of 4000 time steps using a thermostat target temperature of 2000K, the interaction between the BN molecule and the surface of the B liquid could be studied. Repeated simulations of this kind can be repeated to form a BN flake on the surface, which can then begin to fold onto itself and form a nanotube.
- Past simulations[5] have successfully synthesized BNNTs without root-growth mechanisms, so we moved onto bombarding a designed nanostructure grown on a B liquid drop.
- We originally sought to bombard a double-walled BNNT with hydrogen in order to study the interactions between hydrogen and these double-walled BNNT, but we chose instead to bombard single-walled nanotube with hydrogen to create holes.
- Nanotube was taken from previous simulations carried out by Longtao, liquid Boron drop was added manually, and the end of the BNNT was fixed with hydrogen.



FUTURE WORK

- Studying the development of a BN flake on a boron droplet and the folding thereof into a nanotube.
- Hydrogen bombardment on a double-walled BN nanotube.
- How long a nanotube can be grown given that the base or root is bombarded with BN molecules.

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