Integrated multi-scale study for nanosynthesis in plasma volume
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Motivation

High flux of active contents (atoms, ions and electrons) in plasma volume suggest different growth mechanisms from other approaches. To obtain a better understanding of the growth mechanisms in plasma, we conduct multi-scale computational calculations and simulations, specifically addressing following issues:

- Develop evolution process of the plasma and growth of nanomaterials, in terms of their physical and chemical properties
- Recommend optimal plasma parameters for controlled synthesis

Methodology

**CNT**
- First principle density functional theory (DFT) approach is used to analyze many properties such as the energy of binding adatom states, the activation barriers, reaction paths and electron density.
- Kinetic Monte Carlo (KMC) simulation is performed to find lifetime of active adatom and distance of adatom migration.

**BN**
- Quantum classical molecular dynamics (MD) code (SCC-DFTB) is implemented to simulate the growth of boron-nitride nanocages, fuller-renes and nanotubes.

Migration of carbon adatoms at SWCNT surface

**Ultimate problem:**
Can migration of adatoms over the external surface of SWCNT feed the tube growth in plasma?

- In previous model$^1$, only catalyst surface can provide C atom for growth, because C comes from hydrocarbon molecules.
- Plasma environment can provide active C atoms, which can also be captured on CNT surface.

**Theory:**

- Migration of adatoms can be described by diffusion theory. All needed properties can be calculated.
- Migration of adatoms terminates with desorption. Its probability can be described by adsorption energy (Ea).
- Charging on CNT can affect the migration and desorption.

**Results:**

- Migration with small energy barrier exists in (5,5) chirality type, along the nanotube axis direction.
- With increase of charge on CNT, adsorption energy increases while migration barriers remain similar values.
- Carbon atom adsorbed on CNT surface can migrate efficiently through fast migration path. Migration distance increases with increase of charge.

Growth of BN nanostructure

In this project, different approaches are tested to simulate the growth of boron-nitride nanostructure.

- Classical MD: LAMMPS
- Quantum classical MD: SCC-DFTB

**BN fullerene:**
- Boron cluster with different sizes: 36, 96 atoms

**BN “graphene”:**
- HBNH is used as feedstock molecule. BN “Graphene” can be built with B6 cluster as seed or without seed.
- H atoms terminate the boundary of BN nanostructure, which prevents it building into cage.

**BN nanotube:**
- For the first time, the simulation of BNNT growth is achieved.
- A 0.7nm zigzag type BNNT grows to 2nm under continuous bombardment of BN molecules

**Conclusion:**
- SCC-DFTB is a successful approach to simulate growth of BN nanostructures.
- Seed and feedstock species, temperature, pressure and flux can all affect the structure of product.

**References**


Acknowledgement:
Results in this research were obtained using the high-performance Lired computing system at the Institute for Advanced Computational Science of Stony Brook University, which was obtained through the Empire State Development grant NYS #28451.