Shaping nanotubes with an electron nano-beam.

Theoretical and experimental aspects

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1. HREM observations [1]

Direct imaging of single point defects induced by electron irradiation on single walled BN nanotubes.

(a) before irradiation  (b) after 20 s of irradiation: bright spots appear associated with a small decrease in the tube diameter.

2. Defect migration [2]

2.1 Migration path

DFT relaxed structure of a single and a divacancy in a (14,0) BN nanotube and corresponding HREM simulated images.

More extended defective structures are also observed.

(a) before irradiation  (b) after 20 s of irradiation: a kink appears.

DFT relaxed structures of a dislocation line in a BN nanotube and corresponding HREM simulated images. Kinks are associated with dislocation lines along the tube axis.

2.2 Activation energies

Gibbs free energies including vibrational energy and the entropic term have been calculated. Along the migration path nonequivalent structures have different vibrational spectra and consequently different \( \Delta G \) temperature dependence.

3. Electron nanolithography [1]

The graph shows that once a vacancy forms, the formation energy for a subsequent neighboring vacancy is close to zero; thus the probability of forming a second neighboring vacancy is higher than at any other site. This strong driving force suggests that vacancies in single-walled boron nitride tubes will tend to appear as boron-nitrogen pairs.

The intrinsic defects studied here introduce additional states into the gap. Single vacancies introduce half-filled shallow acceptor states and thus may be expected to act as electron acceptors. The electronic structure of the neutral divacancy is different from that of the filled shallow state.

4. Electron nanolithography: Knock on cross section [3]

The theoretical cross section for Coulomb scattering between a relativistic electron and a nucleus have been estimated by Mott as a function of the incident electron energy. The total displacement cross section can be obtained by integrating the cross section inside the energy domain over which emission energy is above a certain emission threshold.

The map of the atomic emission energy threshold for a graphene layer as obtained by DFTB extended molecular dynamics simulations.

Total knock-on cross section for carbon atoms in a single walled carbon nanotube as a function of their position around the tube circumference and incident electron energy. These cross sections give the number of electron required to sputter atoms in the tube.


Using a dedicated STEM microscope with experimental conditions optimised on the basis of derived cross-section, we have been able to control the generation of defects on nanotubular systems. Either, points and line defects can be obtained with a spatial resolution of few nanometers.

References


