MDSPASS2 Tutorial 2

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Note: Use the binary version from 201506xx.

1. Creating the Structure of a Carbon Nanotube (CNT)

1.1. In the **Control Panel**, if the **File Control and Config Creation** section is not yet expanded, click it to roll it out. Then click **Create Config** to open the corresponding panel.

1.2. Now create the CNT structure:

- In the **Atom** field, type **C** and press the **Enter** key.
- For the **Potential**, select **Brenner**.
- Select **Nanotube** from the radio button options.

1.3. In the upper right fields labeled **# of rep in x/y/z**, enter **1, 1, 20**, respectively. This will generate a nanotube structure with the length equivalent to 10 unit cells in the **z-direction** (CNT axis).

1.4. In the **mof(m,n)** and **nof(m,n)** fields, input the **chiral vector** for the CNT (refer to Figure 1). For a narrow **zigzag-type** CNT, set **m = 8, n = 0**.

1.5. The **NT cell size (x/y)** fields specify the simulation cell size perpendicular to the CNT axis, in **angstroms**. Enter **50** (or any value large enough to enclose the CNT diameter; since periodic boundary conditions won't be applied in x and y, this is generally sufficient).

Note: Since the structure is defined as a nanotube, the **nearest-neighbor distance** is automatically set to the experimental graphene value of **0.142 nm**, so the **Lattice const. field** can be ignored.

1.6. At the bottom of the panel, click **Create**. The CNT structure will appear in the **MD Viewer** window. Then click **Close** to exit the panel.

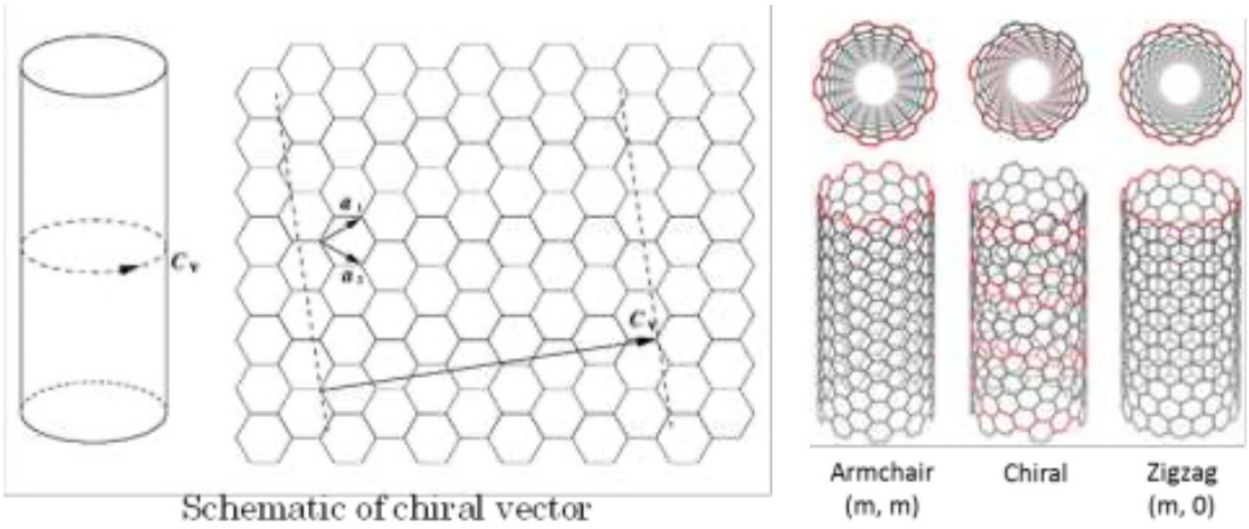

Figure 1 – **Chiral vector** C_v representing the structure of a carbon nanotube (CNT). It is expressed in the form of (m, n), where $C_v = ma_1 + na_2$ and a_1 and a_2 are the unit vectors of the graphene lattice.

2. Compression Analysis of the CNT

2.1. Set Boundary Conditions

- Assuming the CNT structure has been created:
- In the **Control Panel**, uncheck **PBC x** and **PBC y**, and check **PBC z**.
- This applies periodic boundary conditions only in the **z-direction** (the CNT axis).

2.2. Set Visualization Parameters

- Click **Set param** to open the **Set Parameters** panel.
- Roll out the **Setup for drawing**.
- Check the **Draw bond** and set **Bond length = 1.6 Å** (longer values may incorrectly connect second-nearest atoms, leading to clutter and slower rendering).
- Uncheck **Draw Force** for clearer viewing.
- Set **Sphere radius = 4**, **Sphere segment = 8**.
- Roll out **Atom color**, select **Energy**, and check **Autorange**.

2.3. Set Simulation Parameters

- Set **Relax algo = GLOC**.
- Roll out **Deformation settings**, and confirm **ex = ey = ez = 0**.
- Click **Close** to exit the panel.

2.4. Initial Structure Relaxation

- Set **Algorithm = Relaxation (atom)**.
- Click **MD on/off** to run the relaxation calculation. Running ~100 steps should suffice.

2.5. Compression at Finite Temperature

- In the **Temp set** field, enter a desired temperature (e.g., **100 K**).
- Set **Algorithm = NVT** to run a constant temperature MD simulation.
  (Random initial velocities are assigned based on the Boltzmann distribution.)
- Set the timestep **dt = 1.0 fs**.
- Click **Set param**, roll out **Deformation settings**, and set **ez = -0.02** (compression strain rate along z).
- Uncheck **Repeat Lz**.

2.6. Start Compression Simulation

- Click **MD on/off** to begin the compression MD simulation.
- As the simulation progresses, the CNT will start bending into an **S-shape**, and later buckle into a **sharp fold**. This unstable deformation is referred to as **buckling**.
- You may stop the simulation by clicking **MD on/off** again.

2.7. Resetting the Structure

- Clicking **Reset** restores the structure to its original (post-creation) state. Use this if the compression fails or if you wish to test modified conditions.

3. Observing the Post-Buckling State

3.1. With MD paused, use the **Rotation, ObjectsXY, and ObjectsZ** controllers in the **Control Panel** to observe the structure from different angles. You will notice that atoms in the bent region are color-coded differently, indicating elevated energy levels.

3.2. Look for regions where **bond reconstructions** have occurred — e.g., where 6-membered rings have changed into 5- or 7-membered rings.

3.3. If the viewpoint becomes too difficult to navigate, click the **MD Viewer** and press **`r`** to reset the view.

4. Post-Buckling Tension Simulation

4.1. Open **Set Parameters** and in **Deformation settings**, set **ez = +0.02** (tensile strain rate along z).

- Make sure **Repeat Lz is unchecked**. If it's enabled, the strain sign will reverse to keep Lz between min and max.

4.2. Click **Close**, and then click **MD on/off** to begin tensile MD simulation.

- The previously bent CNT will stretch and may return to its original shape.
- Reconstructed bonds (e.g., forming 5- or 7-membered rings) may revert to 6-membered rings, though not always.
- This shows CNTs are highly flexible and can absorb strain via bond reconstructions, exhibiting **reversible deformation** behavior.

5. Buckling Analysis Under Various Structures

5.1. Repeat Sections 1–3 with different CNT structures to observe how buckling behavior changes. For example, setting the chiral vector to **(20, 0)** creates a large-diameter CNT.

Note: In cylindrical shell buckling, increasing the diameter (i.e., lowering aspect ratio) results in different buckling modes. Rather than **S-shaped (Euler) buckling**, you may observe **drum-can-like buckling**, also called **lantern-type** or **diamond-type** buckling.

5.2. Try running **zero-temperature** buckling simulations:

- Keep **Algorithm = Relaxation** and start compression.
- Even for slender CNTs, **Euler buckling may not occur** due to the lack of thermal fluctuations.

  Note: In the absence of thermal fluctuation, the system may reach an unstable equilibrium without buckling. (See Figure 2.)

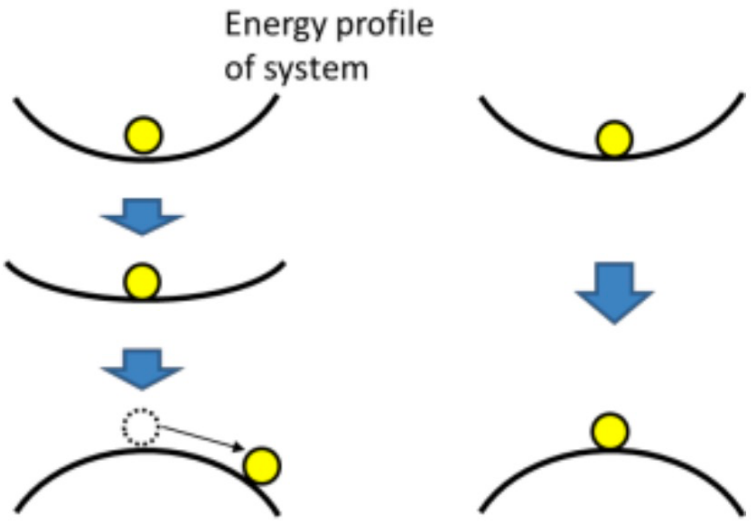

Figure 2 – Schematics of structural destabilization and unstable equilibrium.