mdspass2 Tutorial and Exercises

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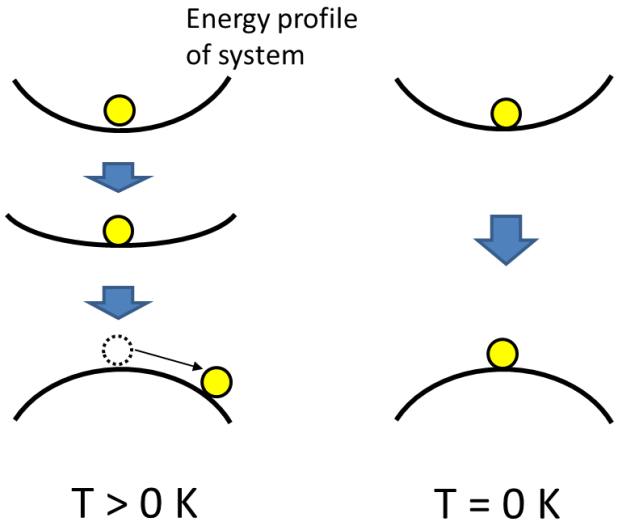
Part III: Deformation of Structures

1. Creation of Nanowire Model and Tensile Simulation

   Let us create a Cu nanowire model and perform tensile MD simulation.

   1. Open the Create config panel, set Atom = Cu, Potential = EAM Mishin, and select FCC as the structure. Set # of rep in x/y/z = 3, 3, 8, and Lattice const. = 3.61. Click Create and then Close.
   2. Open the Set parameters panel. Check Draw bond and set Bond length ≈ 2.8. Set Relax algo = GLOC. Open Deformation settings and confirm that ex = ey = ez = 0; if not, set them to zero. Close the panel.
   3. In the Control panel, set the Potential ARG to Mishin. Uncheck PBC x and PBC y, and check PBC z. This applies periodic boundary conditions only along the z-direction, creating a nanowire configuration.
   4. Set dt ≈ 2.0, choose Algorithm = Relaxation (atom), and run MD for several hundred steps. (The structure will contract slightly in the x and y directions.)
   5. In its current state, the structure is nearly a perfect ideal lattice. If tensile or compressive deformation is applied directly, the structure may resist deformation due to being in an unstable equilibrium (see figure).

      To introduce slight "initial imperfections," set Temp set ≈ 300, choose Algorithm = NVT, and start MD. After the atoms begin to vibrate, run MD for several hundred steps and then stop. Switch Algorithm back to Relaxation (atom) and run MD again for structural relaxation (a few hundred steps is sufficient). Although the structure appears almost unchanged, this sequence (finite-temperature MD + relaxation) introduces small imperfections that facilitate deformation.

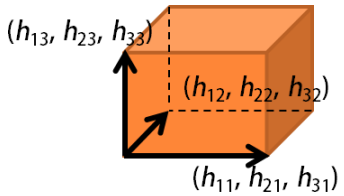


図：構造不安定化と不安定平衡のイメージ。

6. Using the relaxed nanowire, open Set parameters, change Relax algo to FIRE (FIRE accelerates relaxation by dynamically adjusting timestep; see Bitzek et al., PRL 97 (2006) 170201). Under Atom color, select CSP, uncheck Autorange, and set min = 0, max = 0.03 (suitable for visualizing stacking faults). Under Deformation settings, set ez ≈ 0.002, uncheck Repeat Lz, and close the panel.
7. Ensure Algorithm = Relaxation (atom) and run MD. The nanowire stretches in z, and after some time, a sudden structural transformation occurs. With slower strain rate and larger imperfections, dislocations would nucleate from the wire edge, but here the strain rate is high and imperfections small, so a transformation-like collapse occurs.
8. To introduce a larger imperfection, open Create config, roll out Edit config, left-click to select an edge atom in the MD viewer, and press Remove atom. Close the panel.
9. Now, let us extend to cyclic tension/compression along z. Open Set parameters, roll out Deformation settings, check Repeat Lz, set Lz(min) = 30.0, Lz(max) = 34.0, then close the panel. When MD runs, the sign of ez automatically reverses whenever Lz reaches its minimum or maximum, producing cyclic tension and compression between these bounds.
10. Start MD. Just before Lz reaches 33 Å, slip deformation should initiate near the location where the atom was removed. Because the strain rate remains high, transformation-like behavior may appear, but slip-type patterns can be recognized. Adjusting Lz(min) and Lz(max) changes the behavior, so try different

ranges.

11. During MD, stresses are written to stress.d in the format: step, $\sigma_x, \sigma_y, \sigma_z, \tau_{xy}, \tau_{yz}, \tau_{zx}$. Cell sizes are written to cell.d in the format: step, $h_{11}, h_{21}, h_{31}, h_{12}, h_{22}, h_{32}, h_{13}, h_{23}, h_{33}$ (see figure).



2. Construction and Compression of a Carbon Nanotube (CNT)

<Model Construction>

1. Click Create Config, and from the Create config panel, construct the CNT structure. Set Atom = C and Potential = Brenner. From the radio buttons below, select Nanotube. In the # of rep in x/y/z fields at the upper right part of the panel, enter 1, 1, and 20, respectively. This will create a nanotube structure whose length corresponds to 20 unit cells along the z-direction (the CNT axis).

   Note: The axial size of the unit cell depends on the chiral vector (see below). For chiral CNTs (n ≠ 0 and m ≠ n), the unit-cell length is generally large.
2. In the fields m of (m, n) and n of (m, n) below that, enter the chiral vector of the CNT (see the figure for an explanation of the chiral vector). Here we will construct a thin zigzag-type CNT. Set m = 8, n = 0.
3. In the field NT cell size (x/y) below that, specify the cell size in the directions perpendicular to the tube axis in angstroms. Any value sufficiently larger than the tube diameter is acceptable, so enter, for example, 50. (Since periodic boundary conditions are not applied in x and y, any value larger than the CNT diameter will cause no issues.)

   Also note that when the Nanotube structure is selected, the structure is generated so that the nearest-neighbor distance matches the experimental graphene value of 0.142 nm. Therefore, the Lattice const. field is ignored.

   Click Create at the bottom of the panel. Once the structure appears in the MD viewer window, click Close at the bottom of the Create config panel to close it.

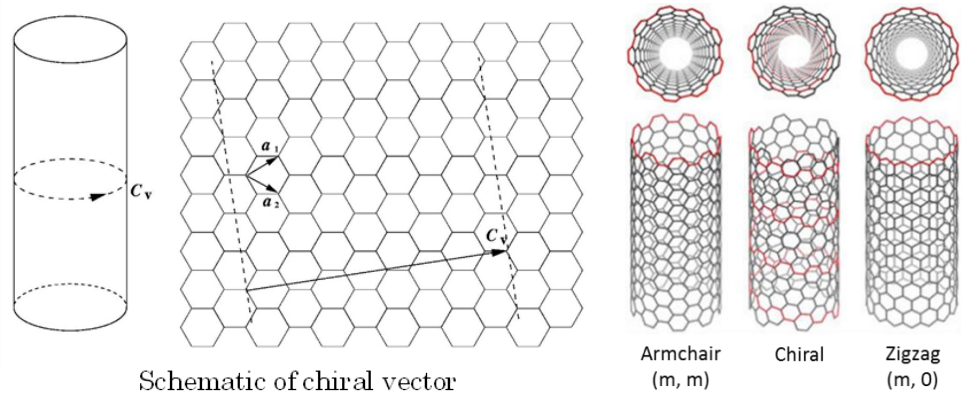


Figure: Chiral vectors representing the structure of a CNT. They are expressed in the form (m,n), and given by $C_v = ma_1 + na_2$. When $n = 0$, the CNT is called *zigzag*-type, and when $m = n$, it is called *armchair*-type.

<Axial Compression Analysis>

1. In the Control panel, uncheck PBC x and PBC y, and check PBC z. Periodic boundary conditions will then be applied only in the z direction (the CNT axis).
2. Click the Set param button to open the Set parameters panel. Roll out Setup for drawing, check Draw bond, and enter 1.6 in the Bond length field (if the value is too large, second-nearest neighbors will also be connected, making the display difficult to see and slowing the drawing). It is easier to view the structure with Draw Force unchecked. Roll out Atom color, check Energy, and also check Autorange. The values for Sphere radius and Sphere segment can be chosen freely, but something like 4 and 8, respectively, is appropriate.
3. Set Relax algo to GLOC. Roll out Deformation settings and confirm that the values of ex, ey, and ez are all zero. Click Close to close the Set parameters panel.
4. Set Algorithm to Relaxation (atom) and press MD on/off to perform a relaxation calculation. About 100 steps should be sufficient.
5. Enter the target temperature (for example, 100) in the Temp set field, and set Algorithm to NVT so that the MD calculation is performed under constant temperature. Set the MD time step dt = 1.0. Press Set param to open the panel again, roll out Deformation settings, and enter a negative value (for example, –0.02) in ez. Leave Repeat Lz unchecked. Click Close to close the panel.
6. Press MD on/off to start the compression MD calculation. As the compression progresses, the CNT will bend into an S shape, and with further compression it will bend sharply (“kink”) like the Japanese character “く”. At that point, press MD on/off once to stop the MD calculation. Such bending and kinking are

unstable deformation modes and are referred to as buckling.

7. Pressing the Reset button will restore the configuration to the state right after the structure was created. Use this if the compression MD attempt fails or when you want to slightly change the calculation conditions.

<Observation of the Buckled State>

1. With MD stopped, use the viewpoint controllers in the Control panel (Rotation, Objects XY, Objects Z) to observe the atomic structure from various angles. You will notice that the colors of some atoms in the bent region have changed, indicating that their energies have increased.
2. Also, due to bond rearrangements, you may find locations where six-membered rings have transformed into five-membered or seven-membered rings. Try searching for such regions.

   Note: If you manipulate the viewpoint too much and cannot return it to the original orientation, click inside the MD viewer window and press the “r” key to reset the viewpoint to its initial state.

<Tensile Loading After Compression Buckling>

1. Press Set param to open the panel, and in Deformation settings, set ez to a positive value (for example, 0.02). Again, confirm that Repeat Lz is unchecked. (If it is checked, the sign of ez will be forcibly reversed so that the cell length in the z direction stays between Lz(min) and Lz(max).)
2. Click Close to close the panel, then press MD on/off to start the tensile MD analysis. The previously bent region should gradually stretch and return toward the original CNT structure. Bond rearrangements that produced five- or seven-membered rings should also revert to six-membered rings (although in some cases they may not). From this behavior, we can see that CNTs are special materials with high flexibility: even under very large deformation, they can absorb strain through bond rearrangement and recover their original structure upon unloading.

[Exercises]

1. Tensile and Compressive Deformation of a Nanowire

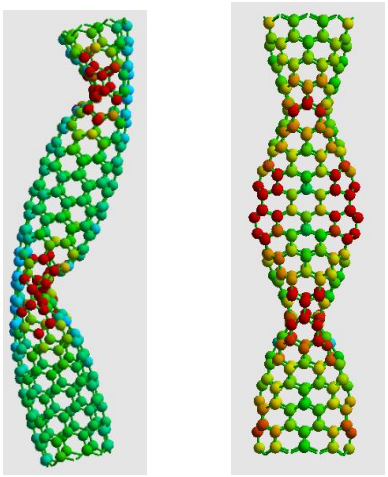
   With reference to the above procedures, perform simulations of simple tension, simple compression, and repeated tension–compression of a nanowire, and describe

the results using snapshots and graphs. Observe, for example, how the stress changes when structural transformations such as slip occur, and how the deformation behavior depends on initial structural imperfections (defects) or strain rate. Try various conditions, such as setting an appropriate temperature and running NVT (constant-temperature) simulations, changing the atomic species (Cu, Al, Si are relatively easy to handle), or varying the wire size.

2. Buckling of CNTs

   Vary the structure and size of a CNT and examine how the buckling deformation changes accordingly. For example, choosing a chiral vector (m, n) = (20, 0) results in a large-diameter CNT.

   Note: In the buckling problem of cylindrical structures, when the diameter is extremely small relative to the length (i.e., when the aspect ratio is large), S-shaped buckling (Euler buckling in strength of materials) occurs; as the aspect ratio decreases, buckling modes similar to the collapse of a drum can appear (often referred to as lantern-type or diamond-type buckling). For CNTs, S-shaped buckling or buckling accompanied by a kink (localized necking) should be observed when the aspect ratio is large, whereas fin-type buckling should appear when the aspect ratio is small (see the figure below).



Kink-type Fin-type

Figure: Examples of buckling deformation of CNT under axial compression.