MDSPASS2 Tutorial

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Note: Use the binary version from 201506xx.

1. Creating a Crystal Structure Model

1.1. In the **Control Panel**, scroll down and click on File Control and Config Creation. This will expand the section and display three buttons: “Config”, “Write Config”, and “Create Config”. Click on Create Config to open the panel.

1.2. Let’s create an aluminum crystal structure. At the top of the panel, you'll see a label “**Atom**” with an input box next to it. Make sure it says **Al**. If not, type **Al** and press the **Enter** key on your keyboard.

1.3. Next, change the **Potential**. Left-click the input box to display the selection menu, and choose **EAM Mishin**.

1.4. Below that, use the check buttons to select the appropriate structure. Since aluminum has an FCC structure, select **FCC**.

1.5. On the right-hand side, you will see input fields labeled **# of rep in x/y/z**. These specify how many unit cells (each FCC cell contains 4 atoms) to stack in the x, y, and z directions. Enter **3** for each. You can type in the values or use the up/down arrows. This will generate a structure with 4 × 3 × 3 × 3 = **108 atoms**.

1.6. Scroll down to the **Lattice const.** input field. Enter **4.04 Å**, which is the lattice constant for aluminum.

1.7. At the bottom of the panel, click **Create**. The crystal structure will appear in the **MD Viewer** window. Then click **Close** at the bottom of the **Create Config** panel.

2. Molecular Dynamics at Finite Temperature

Now, use the aluminum cell (108 atoms) you just created to run a simple MD simulation.

2.1. At the top of the **Control Panel**, you'll find checkboxes for **PBC x/y/z** (Periodic Boundary Conditions in x, y, and z). Since we're simulating a crystal, ensure that **all three** are checked.

2.2. In the **Temp set** field, input the desired temperature (in Kelvin). Enter an appropriate value between **100 and 500**.

2.3. Click **Algorithm** to select an ensemble. Choose **NVT** for constant temperature simulation using the velocity scaling method.

2.4. In the **Status** section below, find the input for **dt (fs)**, the MD timestep in femtoseconds. Enter a suitable value such as **1.0–2.0 fs**. A value that is too significant may cause divergence, while one that is too small will slow the simulation.

2.5. Click **Set param** to open the **Set Parameters** panel. This panel allows various settings including visualization and deformation. Scroll down to **Deformation settings**, and expand it. Ensure that **ex, ey, ez = 0**. Once confirmed, click **Close**.

2.6. Click the **MD on/off** button in the Control Panel to start the MD simulation. You should see atoms vibrating in the **MD Viewer**. Click it again to pause the simulation.

2.7. With the simulation paused, switch the **Algorithm** temporarily to **NVE**, and then back to **NVT**. This will assign initial velocities to atoms based on the target temperature using random numbers.

2.8. The **Status** section in the Control Panel shows information such as step count, average potential energy per atom, temperature, maximum force, and cell size.

3. Adjusting Visualization Settings

3.1. Click **Set param** in the Control Panel to open the **Set Parameters** panel.

3.2. Expand the **Setup for drawing**. Here, you can adjust visualization settings. For example:

- **Ortho** toggles perspective projection.
- **Sphere radius** and **Sphere segment** control atomic size and smoothness. Experiment with the settings.

3.3. If **Draw bond** is checked, atoms within the **Bond length** (in Å) will be connected with lines. For aluminum, try entering **3.2 Å**. If **Bond-PBC** is checked, bonds across periodic boundaries are also shown.
Note: Bonds may not appear immediately after changing the potential or cutoff. Press Calc in the Control Panel to update and render them correctly.

3.4. **Draw force** displays force vectors acting on atoms. Arrow length is scaled by **F-arw length**, which is a scaling factor with no physical unit.

3.5. **Redraw interval** determines how frequently atoms are redrawn. Lower values slow the simulation but yield smoother motion. Try **2** or **10** to observe the difference.

4. Surface Structure Analysis

Let's simulate the structure of a silicon (001) surface.

4.1. Open the Create Config panel from File control and config creation.

4.2. Set Atom = Si, Potential = Tersoff, and select Diamond structure. For # of rep in x/y/z, input 4, 4, 3 respectively. Set Lattice const. = 5.43. Click Create, then Close the panel.

4.3. In the Control Panel, check **PBC x/y** and uncheck **PBC z**. Set **dt (fs) = 2.0**.

4.4. Set Algorithm = Relaxation (atom). Open Set Parameters, set Relax algo = GLOC, and confirm ex, ey, ez = 0. Click Close.

4.5. To make analysis easier:

- Check Draw bond, set Bond length = 3.0
- Set Atom color = Energy, and check Autorange.

4.6. Click **MD on/off** to start the simulation. Run for several hundred steps, then stop by clicking the button again.

4.7. Set **Temp set = 100**, **Algorithm = NVT**, and restart the simulation. After a while, surface atoms will bond and form dimers. Use the **Rotation** controls to observe from different angles.

4.8. Structures may vary due to random initial velocities. If the results are odd, press **Reset** to return to the pre-simulation state and repeat the steps. You can also try changing the temperature or the cell size.

4.9. Once dimer and non-dimer atoms appear, pause the MD and examine atom energies. Click individual atoms in the **MD Viewer**—details will be printed to the **console window**. Dangling bond atoms will have significantly higher potential energy.

5. Nanowire Modeling and Tensile Simulation

Create and simulate the tensile behavior of a copper nanowire.

5.1. In **Create Config**, set **Atom = Cu**, **Potential = EAM Mishin**, and **Structure = FCC**. Note: Using GEAM may provide clearer slip behavior due to its strong preference for perfect FCC.

5.2. Set **# of rep** in **x/y/z = 3, 3, 8**, and **Lattice const. = 3.61**. Click **Create**, then **Close**.

5.3. Open **Set Parameters**, check **Draw bond**, set **Bond length = 2.8**, choose **Relax algo = GLOC**, and ensure **ex/ey/ez = 0**. Close the panel.

5.4. In the **Control Panel**, uncheck **PBC x/y**, and check **PBC z**—this enables a 1D nanowire.

5.5. Set **dt = 2.0**, **Algorithm = Relaxation (atom)**, and run the simulation for several hundred steps using **MD on/off**.

5.6. Set **Temp set = 300**, **Algorithm = NVT**, and **run MD**. Atomic vibrations will begin.

5.7. After several hundred steps, **pause the MD**. Switch to **Relaxation (atom)** and **run MD** again for structural relaxation. Atomic motion will nearly cease, though minor imperfections remain.

5.8. Prepare for tensile simulation.

- Open **Set Parameters**
- Switch **Relax algo = FIRE**
- Set **Atom color = CSP**, uncheck **Autorange**, set **min = 0, max = 0.03**
- Set **ez = 0.002** in Deformation settings, uncheck **Repeat Lz**, then **Close**.

5.9. Confirm **Algorithm = Relaxation (atom)**, and start MD. Tensile deformation in the z-direction begins. Rapid structural changes may occur due to the fast strain rate and small imperfections.

5.10. To introduce initial defects, open **Create Config**, expand **Edit config**, click an edge atom in **MD Viewer** to select the atom to be removed, and press **Remove atom**. Then **Close** the panel.

5.11. To perform cyclic tension/compression:

- Open **Set Parameters**, check **Repeat Lz**, and set **Lz(min) = 30.0**, **Lz(max) = 34.0**.

5.12. Please start the MD simulation using this setting. Just before the z-direction cell size reaches **33 Å**, a **crystal slip deformation** will initiate from the vicinity of the atom you previously removed. Since the deformation rate is still relatively high, you may also observe **phase transformation-like behavior** in some areas. However, by carefully observing the repeated deformation process, **slip-like behavior** should become apparent.

It may help to adjust the **viewing angle using the Rotation controller** for better visibility. Also, by slightly modifying the values of **Lz(min)** and **Lz(max)**, you may observe different deformation behaviors, so please feel free to experiment with various settings.