mdspass2 Tutorial and Exercises

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Part II: Surface and Grain Boundary Structures

1. Surface Reconstruction of Si(001)
   1. Click Create Config in the File control and config creation area at the bottom of the Control panel to open the Create Config panel.
   2. Set Atom to Si, Potential to Tersoff, and check the Diamond radio button. Set # of rep in x/y/z to 4, 4, 3, respectively. Enter 5.43 for Lattice const. Click Create to generate the simulation cell, then close the Create Config panel with Close.
   3. In the Control panel, check PBC x and PBC y, and uncheck PBC z. Set dt (fs) to around 2.0.
      This creates a plate-like structure that is infinite in the xy-plane. Such a model is called a slab model.
   4. Set Algorithm to Relaxation (atom). Open the Set parameter panel via Set param, and set Relax algo to GLOC. In Deformation settings, verify that ex/ey/ez are all 0.
   5. For easier structural observation later, check Draw bond, and set Bond length to 3.0. Set Atom color to Energy, and check Autorange. Close the Set parameter panel.
   6. Press MD on/off to start MD. A structural relaxation will be performed. After several hundred steps, press MD on/off again to stop MD.
   7. Next, set Temp set to 100, change Algorithm to NVT, and restart MD with MD on/off. After some time, surface atoms will form bonds and produce dimer structures. Use the rotation controllers in the Control panel to observe the structure from various angles.
   8. The exact structure obtained depends on factors such as the initial atomic velocities (randomized). If the structure becomes unphysical, press the Reset button at the bottom of the Control panel to return to the state before MD. You may also try different temperatures or cell sizes.
   9. When both dimer-forming atoms and non-dimer atoms appear, stop MD with MD on/off. Because their energies differ significantly, they should appear in different colors. Move the mouse cursor over the atoms in the MD viewer window and left-click them (rotate the model or use perspective mode so atoms do not overlap).
      Information about the selected atom will appear in the console window (in Windows, a black text console). This includes the potential energy of the atom.

Atoms not forming dimers have dangling bonds and therefore significantly higher energies.

２. Surface Structure of Al(001)

1. Following the Si example, create an Al(001) surface model. Open Create Config, set Atom to Al, Potential to EAM, and check fcc. Set # of rep in x/y/z to 3, 3, 4. Enter 4.049 for Lattice const., then click Create. Close the panel.
2. In the Control panel, verify that:
   Algorithm = Relaxation (atom)
   PBC x and PBC y are checked
   PBC z is unchecked
   Then, run MD. Rotate the model so the z-axis is vertical; the atoms in the surface layer and the subsurface layer will appear in different colors from the central (bulk) atoms.
3. After an appropriate number of steps, stop MD. Left-clicking atoms will display their information, including coordinates, energy, and stress components. Verify that not only the energies but also the stress components differ between surface atoms and bulk atoms.

３. Construction of a Grain Boundary Model

A (symmetric) crystal grain boundary can be produced by rotating a crystal across a plane and joining the two parts. If the rotation axis is parallel to the boundary plane, the boundary is a tilt grain boundary; if perpendicular, it is a twist grain boundary. Here, we construct a tilt grain boundary.

1. Open Create config, set Atom to Al, Potential to Mishin, and set # of rep to 10, 2, 10. Click Create.This produces a structure extended in x and z but thin in y.
   It is helpful to rotate the view so that the structure is observed from the ±y direction.
2. <Rotating the Model> Roll out Rotation. You can specify rotations around the x, y, and z axes. Enter 30 in the Y field and press Rotate. The atomic structure (and the cell box) rotates by 30° about the y-axis.
3. <Modifying the Cell Box> Roll out Cell dimension. This displays the three vectors of the cell-shape matrix h.
   Check Fix atoms (to change the cell without moving the atoms). Set the diagonal components h13 and h31 to zero.
   Note: Due to a GLUI bug, Enter may sometimes be ignored. If so, enter an intermediate value (e.g., 1), press Enter, then enter the desired value again.
4. <Shifting the Entire Atomic Set> Press Edit atom to open a new popup panel where atomic coordinates can be manipulated. Enter appropriate values and press Shift

all. Here, shift by x = –6.4 Å and z = 4.6 Å.

Note: The editor also allows moving or deleting individual atoms selected by clicking or number input, and adding atoms, but this is not needed here.

5. <Deleting Unwanted Atoms> Roll out Slicer in the Create config window. Atoms with relative coordinates outside the specified x/y/z ranges (0.0–1.0) are deleted. Enter 0.5 for 3 max, then press Slice. Atoms with relative z ≤ 0.5 (the lower half of the cell) remain.

   If atoms remain near the boundary, they may later collide with periodic images. To remove them, set 1 min = 0.02 and 2 min = 0.02, then press Slice again.
6. Write the resulting atomic structure to file by clicking Write Config (in the main Control panel). Rename the resulting file to something like CONFIG.BOTTOM.
7. Repeat the same procedure as above, but rotate the model by –30° (the opposite direction), and then delete the lower half. Save this as CONFIG.TOP.
8. Load the CONFIG.TOP structure (or keep it on screen from step 7). Press Read Config, check Merge, and double-click CONFIG.BOTTOM. This adds atoms from CONFIG.BOTTOM without deleting existing atoms.

   Note: This assumes that the cell sizes of CONFIG.TOP and CONFIG.BOTTOM are identical.
9. Perform a structural relaxation. If atoms are too close, numerical divergence (“explosion”) may occur. Adjust the shift values or the slicing ranges slightly and try again until a stable grain boundary forms.

   10.

[Exercises]

１. Silicon Surface Structure

1) Show snapshots of the Si(001) surface structure as it relaxes from the initial state.
2) Estimate how much the energy changes during this process—that is, the energy change associated with the formation of surface dimers.
3) Determine approximately how many eV per dimer.

２. Structural Relaxation and Surface Energy of Metals

1) Construct an Al(100) surface model and perform structural relaxation. During relaxation, do not relax in-plane stress (i.e., do not adjust the cell size in x–y). Confirm that the interlayer distances parallel to the surface differ slightly from the ideal bulk spacing.
2) Compute the surface energy of Al(100), which is given by

$$\gamma = \frac{E_{slab} - E_{perfect}}{2A}$$

Here, E_{slab} is total energy of the slab model, $E_{perfect}$ is energy of a bulk atom, and A is area of one surface.

Note: $E_{perfect}$ may be computed using a much smaller bulk cell; simply multiply by the number of atoms in the slab.

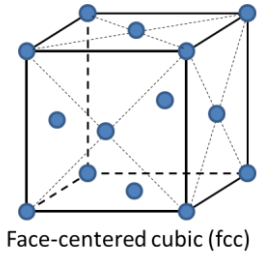
3) Similarly, examine Cu(100). Use lattice constant 3.61 Å and the EAM-Mishin potential.

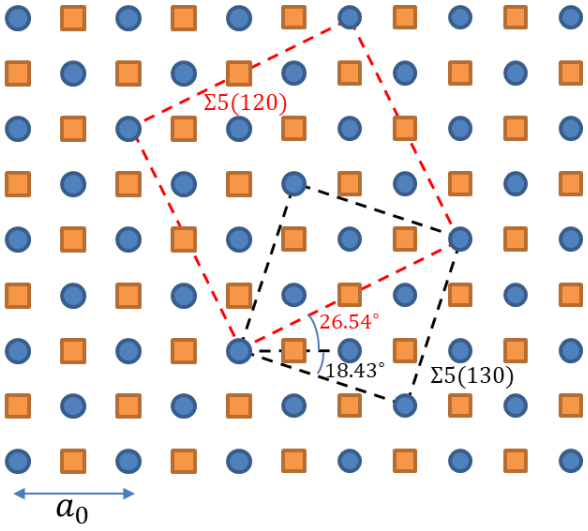
3. Grain Boundary Energy

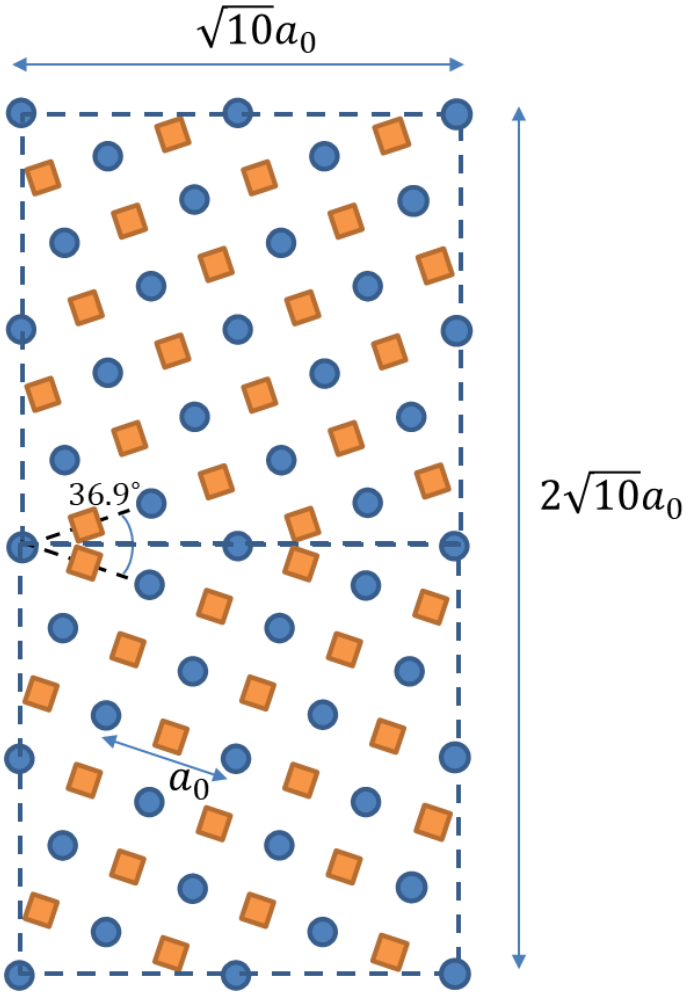
1) Construct a tilt grain boundary model (Al or Cu) and compare the atomic arrangements before and after relaxation.
2) Compute the grain boundary energy.
3) Advanced work (optional): Shift atoms parallel to the grain-boundary plane before relaxation and observe whether the grain boundary energy decreases (a more stable structure).

A schematic example of an fcc tilt grain boundary is shown:

The grain-boundary plane is (120), meaning that when atoms from one grain are projected onto the boundary plane, one in five overlaps with atoms on the other side.







$\Sigma 5(120)$ tilt grain boundary