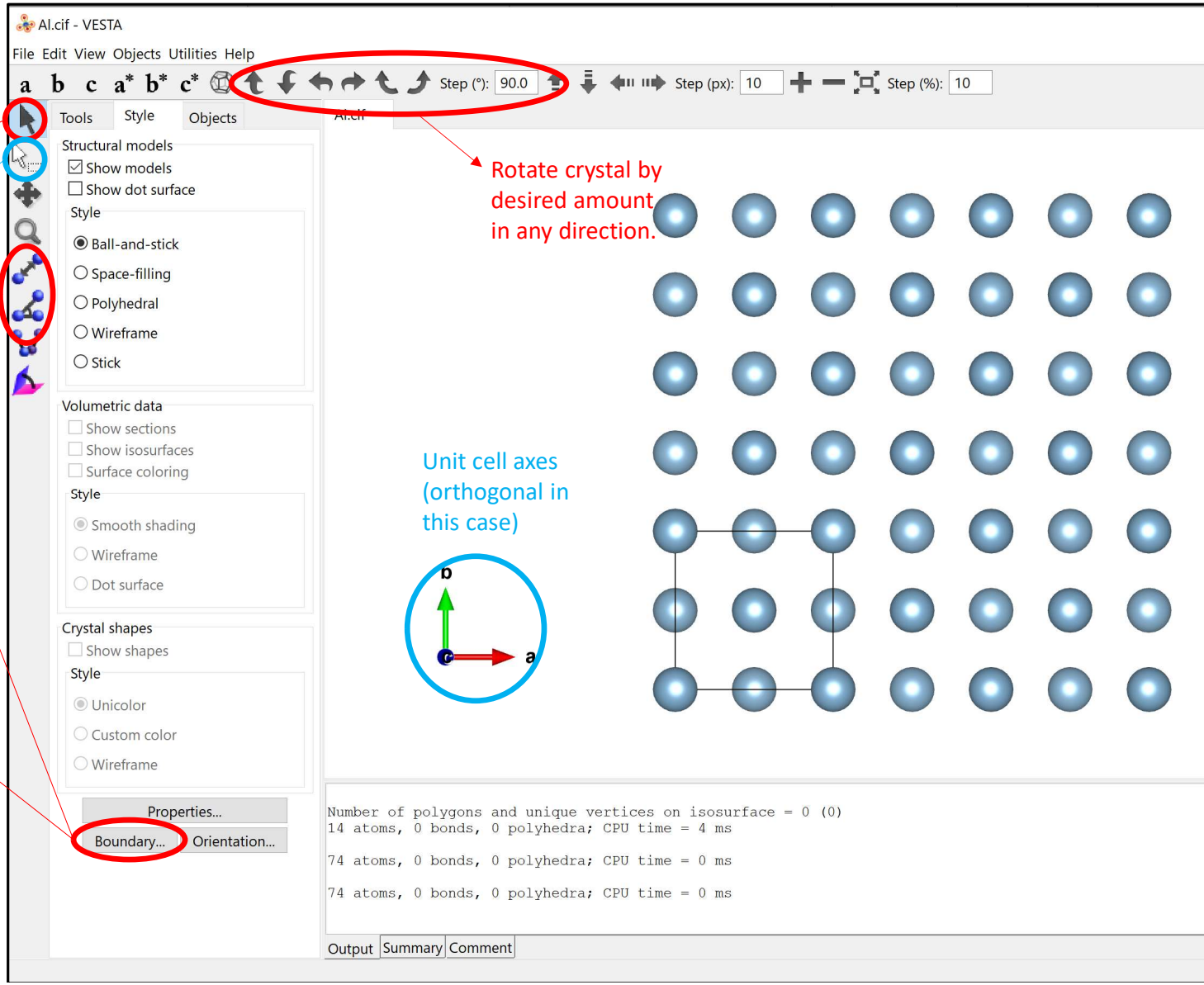
A very, very quick tutorial to Vesta

1. Open Vesta
2. Drag a file into Vesta to open it.
3. See page 2 for how to manipulate the crystal structure.
4. See page 3 for how to find the lattice parameters.
5. See page 4 for how to save a .xyz file.
6. See page 5 for how to open the .xyz file and find individual atomic coordinates.

What you see when you open a structure file.



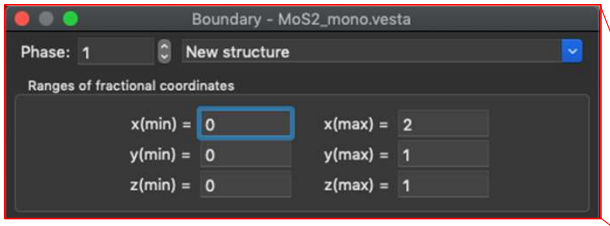
Select individual atoms

Drag box to select a large group of atoms.

Measure distance and angle between atoms.

Rotate crystal by desired amount in any direction.

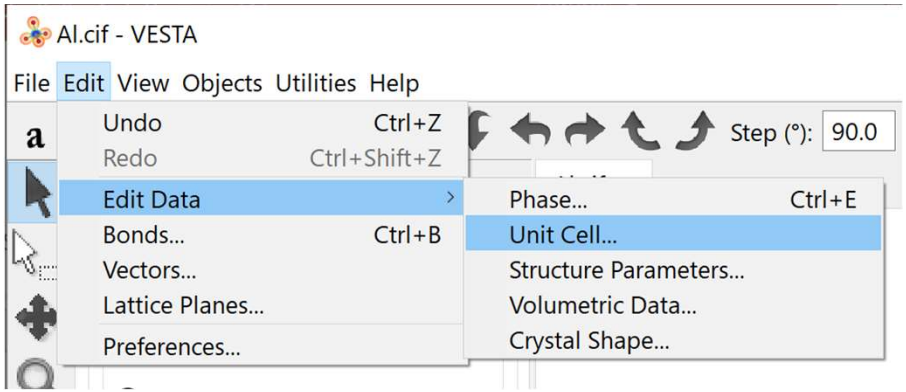
Unit cell axes (orthogonal in this case)



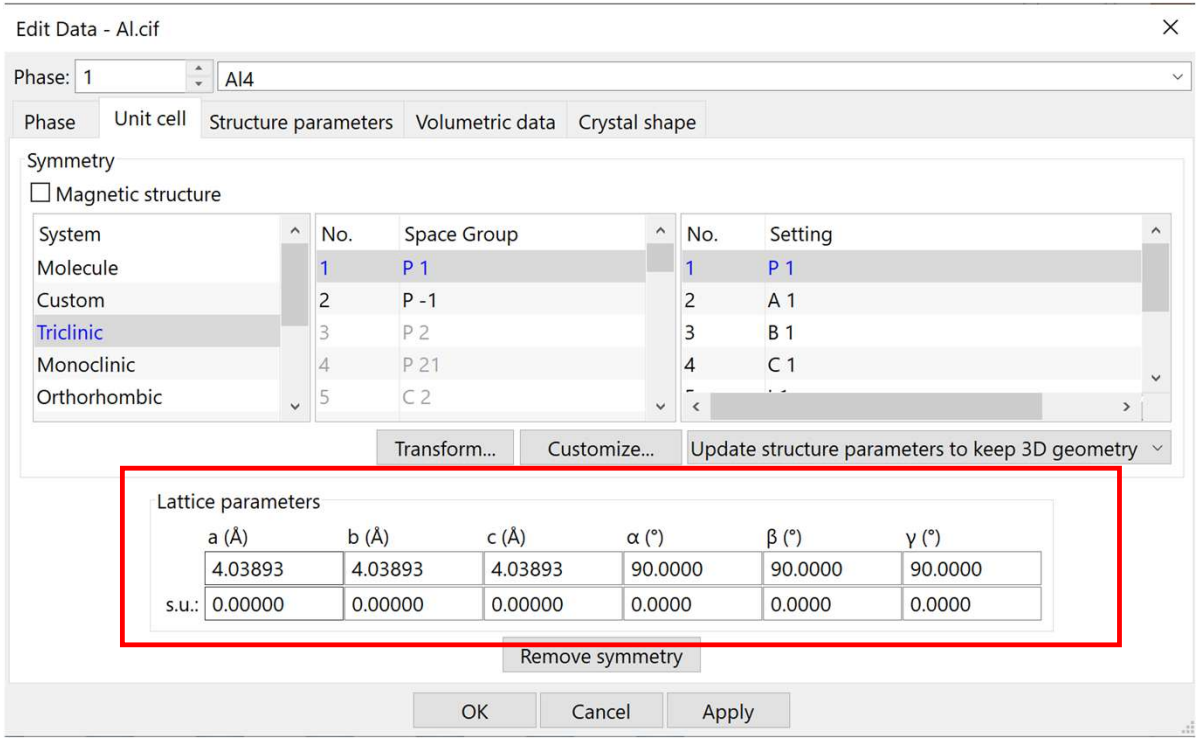
Set number of unit cells in x, y, z directions to make the crystal bigger or smaller.

How to find the unit cell lengths and angles:

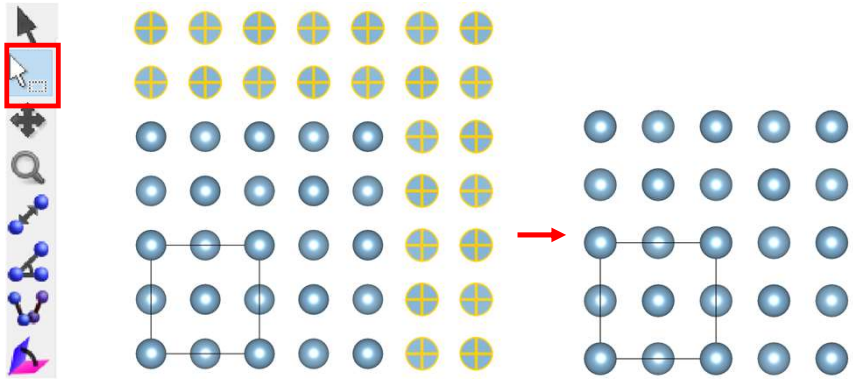
1. Click on Edit → Edit Data → Unit Cell



2. The lattice parameters are listed below:

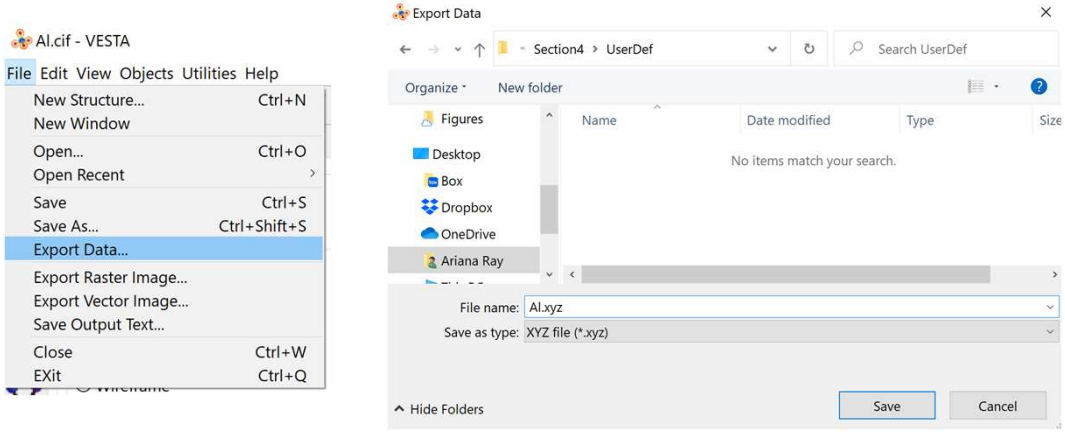


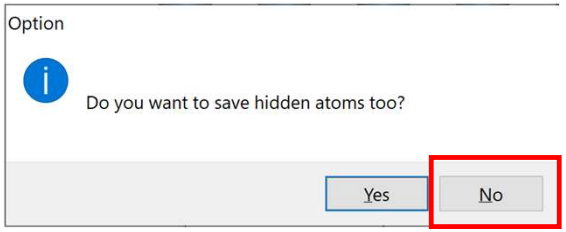
1. Select the atoms you want to remove with the selection tool, then press the delete (not backspace) button to remove them.



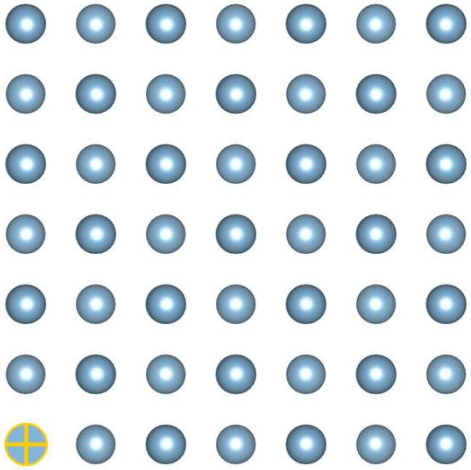
Export a .xyz file

2. Go to File → Export Data → Save as type XYZ file. Hit enter. You'll see a popup asking if you want to save hidden atoms. Say no.





Open .xyz file and find atomic coordinates and occupancy.



Double-click an atom until it's highlighted in yellow. In the bottom of the Vesta GUI, the coordinate of the atom should appear. Repeat for all the atoms needed to tile the unit cell. The .xyz file saves (x,y,z) coordinates while the .vesta file saves fractional coordinates. The (x,y,z) coordinates are more helpful if you have to reshape the unit cell.

```
  74 Al  Al74       10.09732   10.09732    4.03893    1.000    1.000    1          -
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
74 atoms, 0 bonds, 0 polyhedra; CPU time = 1 ms

Atom:  2   Al2 Al  0.00000   0.00000   4.03893   ( 0, 0, 0)+ x, y, z
           Occ. = 1.000       Ueq = 1.00000      1         -
```