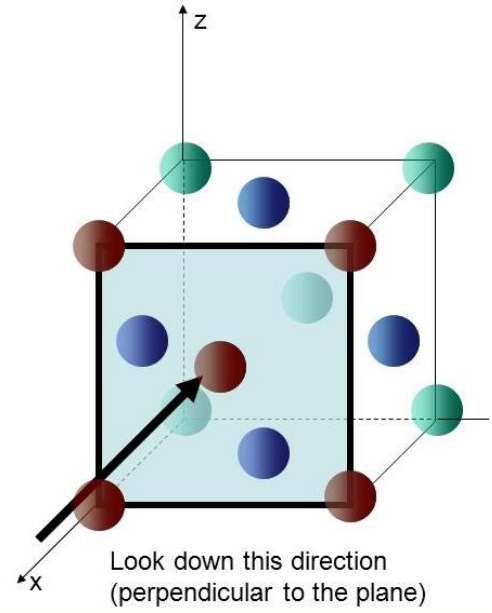
ASESMA 2018 - Worksheet 5
Coordinates of FCC(100) Surface Slab



- Consider Al whose bulk crystal structure is FCC with a lattice constant, a = 4.05 Å.
- Draw the 2D arrangement of atoms on the topmost layer of its (100) surface.
- Mark a length scale in units of a
- Draw two Primitive Lattice Vectors.
- What is the surface lattice constant, '**alat**', in units of a?
- Draw the boundaries of a primitive unit cell.

- Use a new coordinate system where the z axis is perpendicular to the surface (formerly the x-axis). Choose directions for your new x and y axes that are convenient (you have some freedom here, but some choices will make your work easier!)
- What is the interplanar distance in units of **alat**?
- Get the x, y, z coordinates of the atoms in the first five layers in units of **alat**.
- Now, add a vacuum with a thickness equivalent to 6 atomic layers.
- Will the Bravais lattice type now be simple cubic, FCC, tetragonal, or orthorhombic? What is the value of **ibrav**?
- How many parameters (**A**,**B**,**C**, **cosAB**, **cosBC**, **cosAC**) do you need to provide to define the cell? Give their values. For **A** or **B** or **C**. give the value in angstroms.
- When relaxing interplanar separations do you think you need to allow atoms to move in all three directions?

- You will use this to make an input file for an Al(100) surface slab and then do a relax calculation in PWSCF to optimize the interplanar separations.