Properties of Materials
Home Work 2 (Due: 10/06/2010)

1. This question requires you to use an ERC OCC computer. You will need to take four print outs for this question, marked by (a), (b), (c) and (d) below. You will be expected to acquire basic expertise in generating essential crystal structures using the software and hence exploring Materials Studio to understand crystal structure is encouraged.

 (5x4)

Go to OCC>Login>All Programmes> Accelrys Materials Studio 5.0> Materials Studio;

1. Press OK for file association>Create new project: OK>Create new project by your “username” name
2. Structure folder- default: OK>Use Import >Structures>metals>pure metals>
3. Select (a) Cu to open copper unit cell (FCC)>Use right click on corner atom>select Display style>Chose Ball and stick (default is OK)>Close menu:
4. Observe by rotating using rotation tool (as shown below)>Go to edit> **print/copy** (a).
5. Build>Symmetry>Supercell>Put A = B = C = 3>Create Supercell>Close menu
6. Select Build>Surface>Cleave Surface>Cleave Plane (h k l) = (1 1 1)>Close menu
7. Click rotation tool>Rotate to observe hexagonal close packing face > **print/copy** (b)
8. Import Chromium( Cr) structure >**print/copy** unit cell (c)
9. Make 3x3x3 supercell as before>rotate to observe cubic close packing> **print/copy** (d)
10. **Save** project till end of quarter.



Import Tool

Rotate Tool

Select Tool

1. Demonstrate equivalence of FCC packing along (111) face and hexagonal close packing. Calculate the efficiency (fraction of space occupied) in HCP and FCC crystal structure.

 (20+10+10)

1. Compare and contrast the particle and wave nature of x-rays and electrons using relationships between wavelength, *λ*, wave vector, *k*, momentum*, p*, and energy, *E* for both. (20)
2. Comment on equivalence of Bragg’s law and Laue diffraction equation in brief (using concept of reciprocal lattice vector). (20)