

ESO205 Lab-1

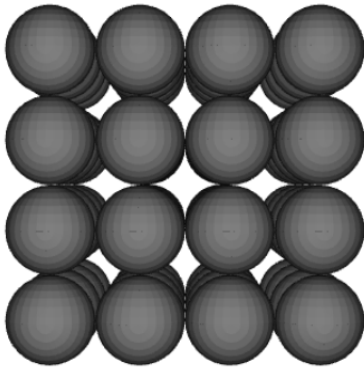
SHUBHAM GUPTA 180749

SEC-3, GROUP-3

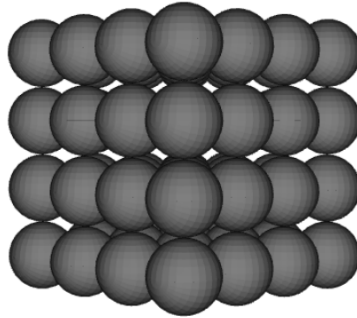
Part A: SC, BCC and FCC crystals from different views

SC Crystal:

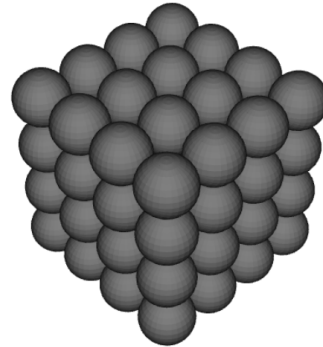
(100)



(110)

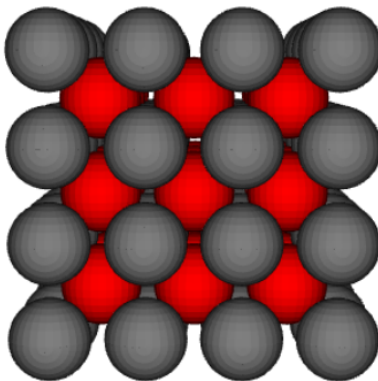


(111)

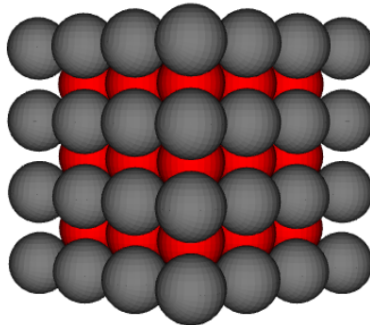


BCC Crystal:

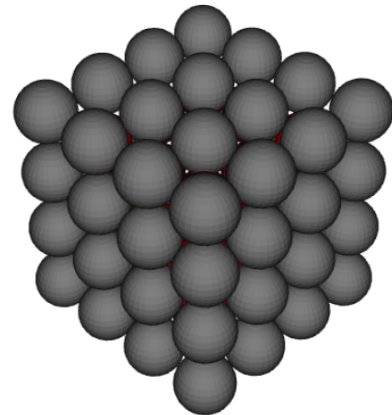
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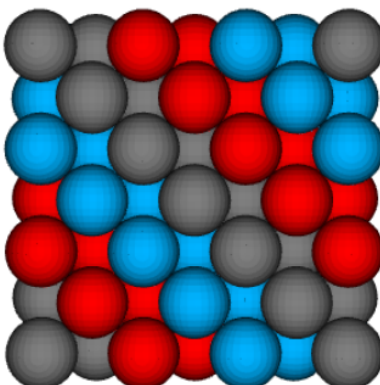


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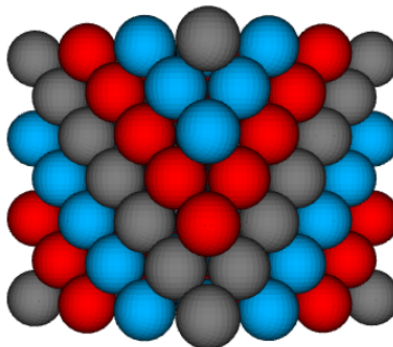


FCC Crystal:

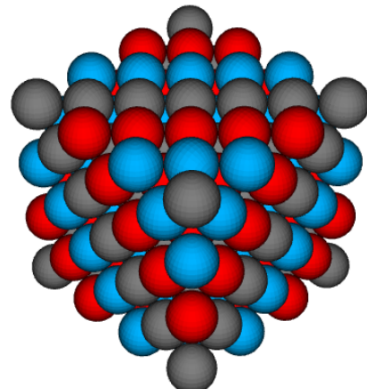
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(110)

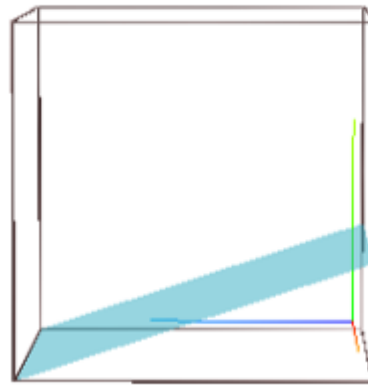
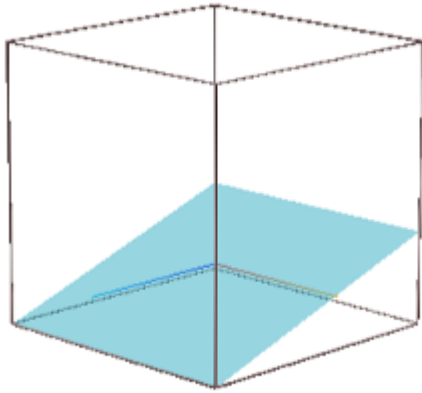


(111)

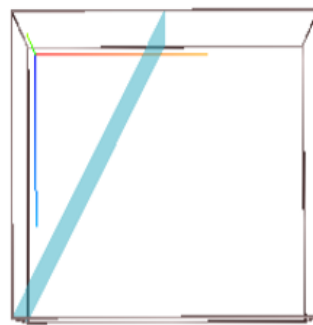
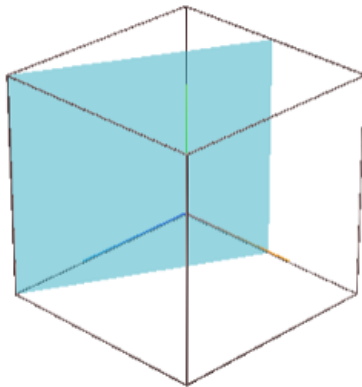


Part B: Visualizing planes using Calistry

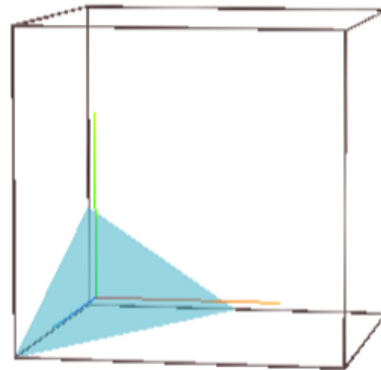
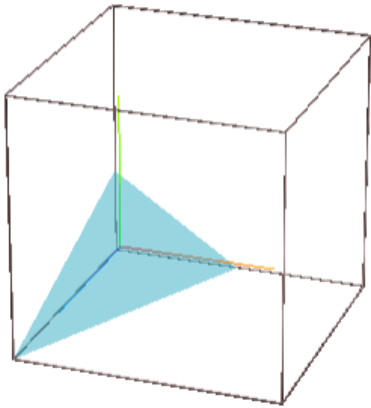
Plane with miller indices $[103]$



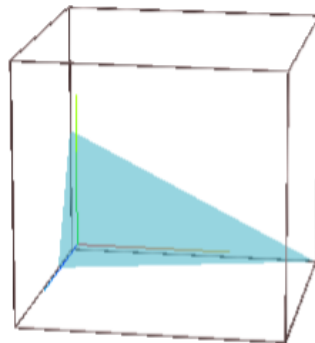
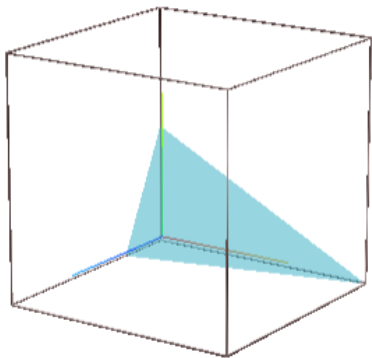
The plane with miller indices $[120]$.



The plane with miller indices $[123]$.

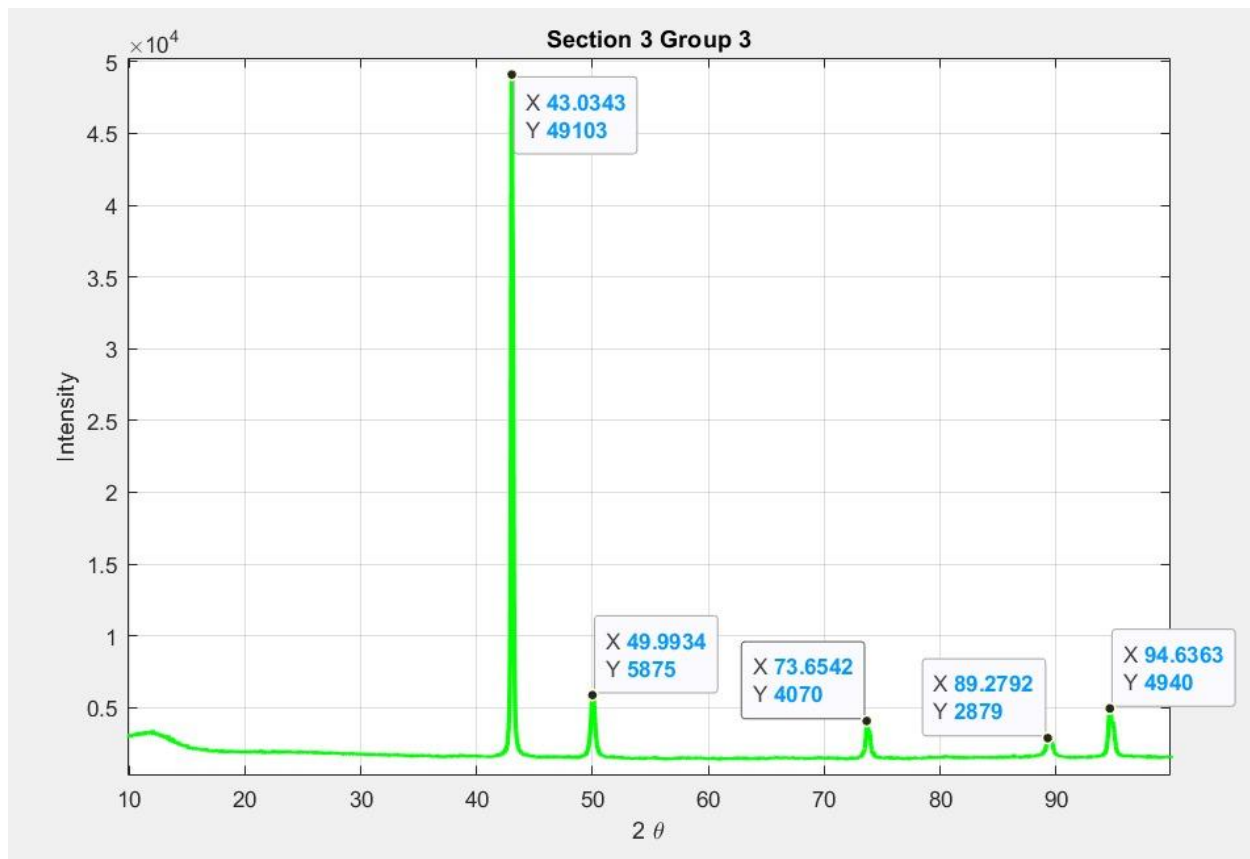


The plane with miller indices $[412]$.



Part C: The crystal structure and lattice parameter for X-ray diffraction pattern

2θ equals 43.0343° , 49.9934° , 73.6542° , 89.2792° , and 94.6363° corresponding to (111), (200), (220), (311) and (222) respectively.



$$\sin^2(\theta_1)/\sin^2(\theta_2) = (h^2+k^2+l^2)/(h^2+k^2+l^2)$$

$$R = \sin^2(21.51715) / \sin^2(24.9967) = 0.753$$

Therefore, this XRD data is FCC.

The first peak in the XRD pattern occurs at $2\theta = 43.0343^\circ$ which is close to 43.2° . Therefore it is copper. Now we use Bragg's law to calculate the lattice parameter.

The lattice parameter comes out to be ~ 3.63 angstroms.

Calculations are in the following table.

λ (Å)	2θ	θ	$\sin^2\theta$	h	k	l	$d = \lambda/2\sin\theta$	$a = d/(\sqrt{h^2+k^2+l^2})$
1.5406	43.0343	21.51715	0.134527353	1	1	1	2.100170719	3.637602389
1.5406	49.9934	24.9967	0.178562076	2	0	0	1.822910239	3.645820478
1.5406	73.6542	36.8271	0.359283075	2	2	0	1.285113596	3.634850153
1.5406	89.2792	44.6396	0.493709999	3	1	1	1.096286172	3.635969896
1.5406	94.6363	47.31815	0.540415211	2	2	2	1.047842757	3.629833785

Error Analysis:

Equate the partial derivative of Bragg's law with respect to d and θ with λ as constant to 0.

$$2 \cdot \Delta d \cdot \sin\theta + 2 \cdot d \cdot \cos\theta \cdot \Delta\theta = 0$$

$$\frac{\Delta d}{d} = -\cot\theta \cdot \Delta\theta$$

From the error equation, as θ increases, the error decreases. This relation indicates to use of the highest peak for lattice parameter for the most negligible error value.

The value of θ will be 47.31815. The corresponding value of the lattice parameter is 3.629833785 angstroms.