

PO SCAR - Au.vasp





Au - ①

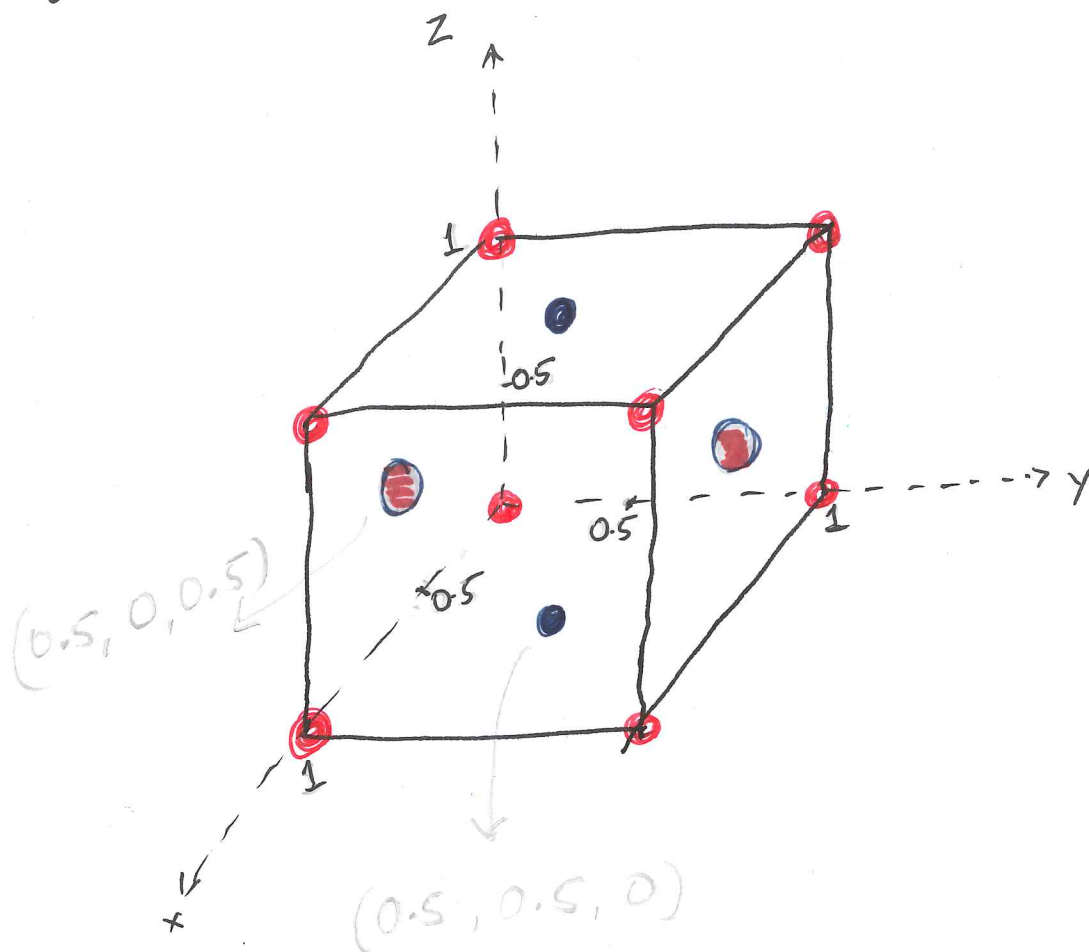
Au  
1.0  
4.0782 0.0 0.0  
0.0 4.0782 0.0  
0.0 0.0 4.0782

- Name of ~~sg~~ material
- Scaling factor (leave it as 1)
- lattice parameter  $a$  (in Å)

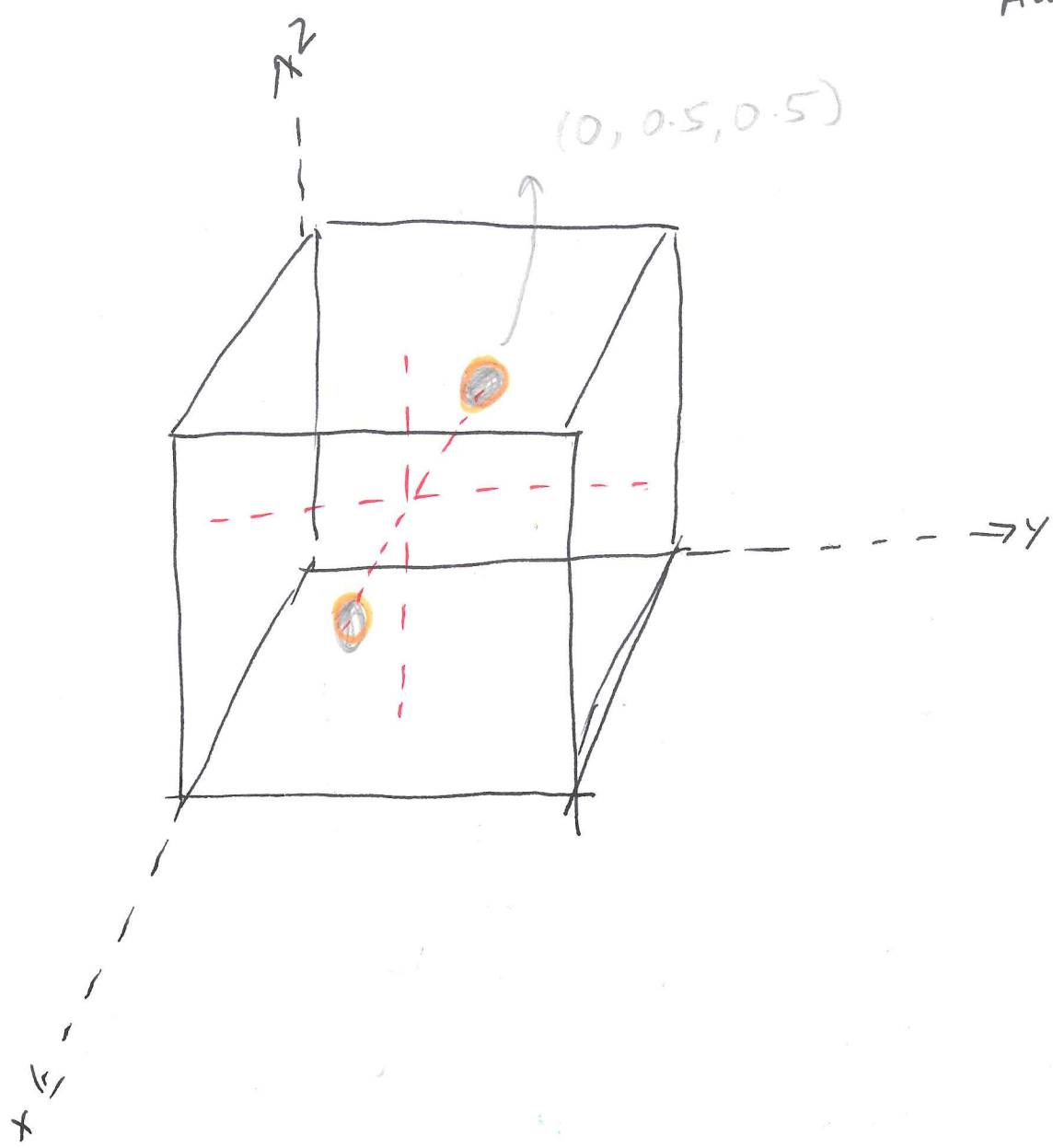
Au  
4  
direct

- Chemical Formula
- No of atoms of Au (We mentioned Au in the last line)
- coordinates of atoms for cell of length 1

0.0	0.0	0.0	Au	
0.5	0.5	0.0	Au	
0.0	0.5	0.5	Au	
0.5	0.5	0.5	Au	



Au - (2)



POSCAR-Fe.vasp

Fe - ①

Fe

1.0

2.867

0.0

0.0

0.0

2.867

0.0

0.0

0.0

2.867

Fe

2

direct

0.0

0.0

0.0 Fe

0.5

0.5

0.5 Fe

z

↑



(0.5, 0.5, 0.5)

↑

1.0

0.5

0.5

0.5

1

y

(0.0, 0.0, 0.0)

x

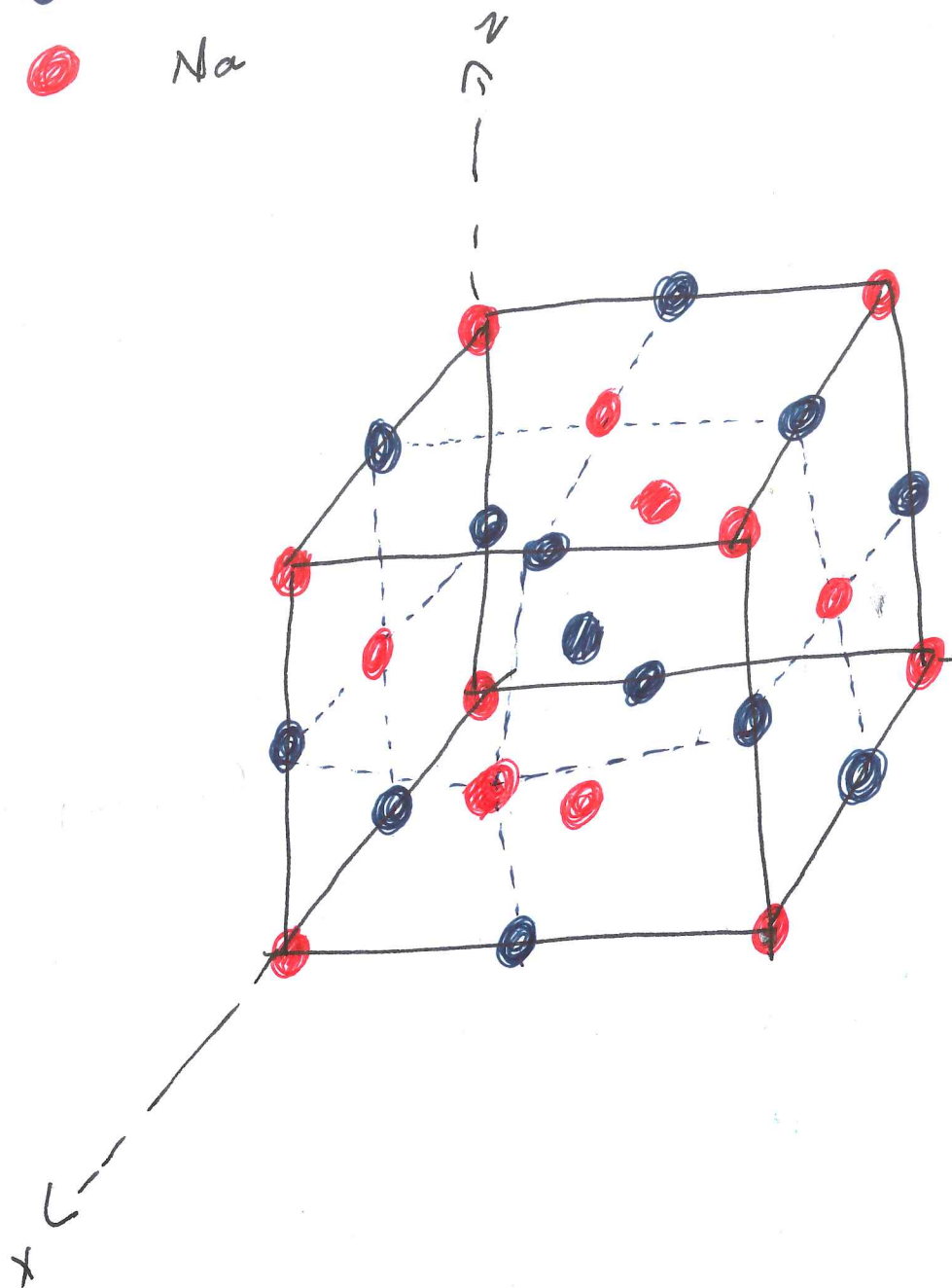


1






 Cl  
 Na

NaCl - (1)



  $(0.0, 0.0, 0.0)$   
  $(0.5, 0.5, 0.5)$   
  $(0.0, 0.5, 0.5)$   
  $(0.5, 0.5, 0.0)$   
  $(0.5, 0.5, 0.0)$

  $(0.5, 0.0, 0.0)$   
  $(0.0, 0.0, 0.5)$   
  $(0.0, 0.5, 0.0)$