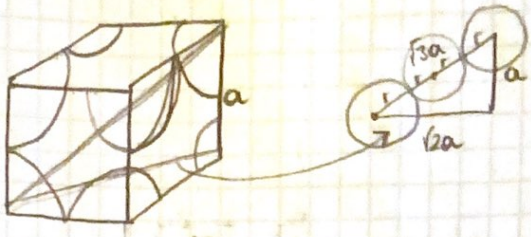
METE Homework 1

Q1) (a) BCC structure w/ lattice param; 0.6080 nm
Atomic radius?



$4r = \sqrt{3}a$

$\frac{a\sqrt{3}}{4} = r$

$a = 0.6080\ nm$

$r = 0.26327\ nm$

Cesium's atomic radius.

(b) lattice parameter = 0.3805 nm
atomic radius = 0.134 nm

FCC

$4r = \sqrt{2}a$

$r = \frac{\sqrt{2}a}{4}$

$0.134 = \frac{(0.3805)\sqrt{2}}{4}$

$0.134 = 0.134$

BCC

$r = \frac{a\sqrt{3}}{4} \rightarrow 0.134 = \frac{(0.3805)\sqrt{3}}{4}$

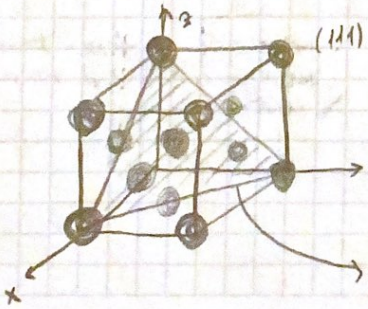
$0.134 \neq 0.16476$

Therefore, Rhodium has FCC structure.

Q2) Atomic packing density for (111) plane of copper.
Linear atomic density along the $[\bar{1}10]$ direction in this plane?

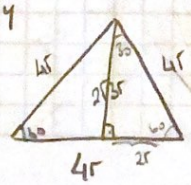
Planar packing factor = $\frac{\text{Area of atom on plane}}{\text{area of plane}}$

Copper has FCC structure



(111) plane on FCC

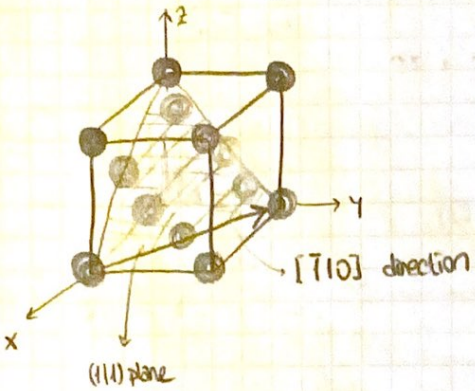
#of atoms centered on the plane = 2

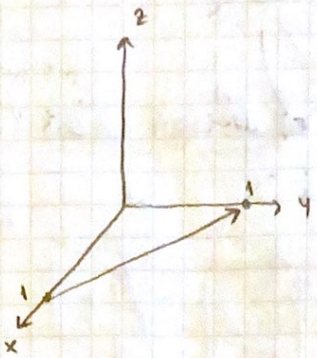


Area of Plane = $\frac{2\sqrt{3}r \cdot 4r}{2} = 4\sqrt{3}r^2$

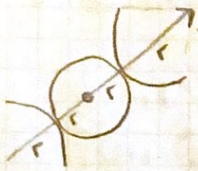
$$\frac{\text{Area of atoms centered on plane}}{\text{Area of plane}} = \frac{2\pi r^2}{4\sqrt{3}r^2} = \frac{\pi}{2\sqrt{3}} \text{ atoms/Å}^2$$

→ Linear atomic density along the [710] direction in this plane?





$$\text{Linear Density} = \frac{\text{Number of atoms centered in the direction}}{\text{Length of the direction vector}}$$



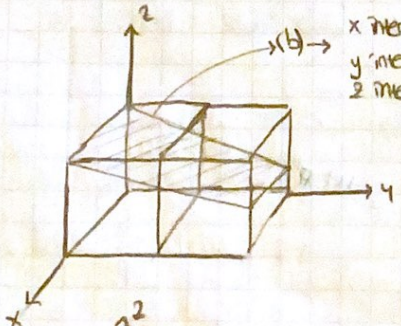
→ 4r ⇒ 2 atoms

length = 4r

copper's atomic radius = r = 1.57 Å

$$\frac{2}{4r} = \frac{2}{4(1.57\text{ Å})} = 0.318\ \text{Å}^{-1}$$

Q3) Miller indices?

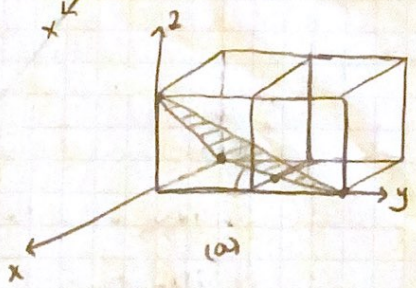


x intercept = ∞
y intercept = 4
z intercept = 1

reciprocals; 0 1/4 1

Reduction; 0 1 4

Miller indices; (014)

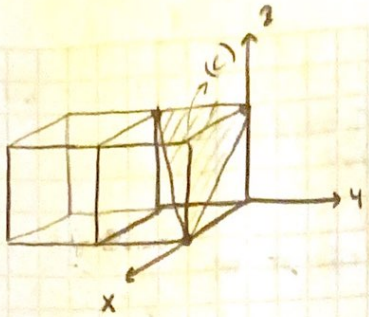


x intercept = -1
y intercept = 2
z intercept = 1

Reciprocals = -1 1/2 1

Reduction = -2 1 2

Miller indices = $(\bar{2}12)$

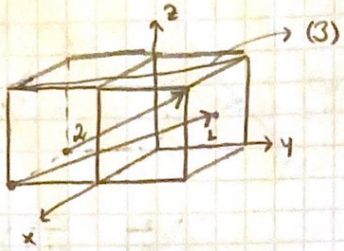


x intercept : 1
y intercept : ∞
z intercept : 1

Reciprocals, 1 0 1

Miller indices (101)

Q4) Miller indices of directions 1, 2 & 3 ?



For (1), head coordinates, $(\frac{1}{2}, 1, \frac{1}{2})$ head - tail = $-\frac{1}{2}, 2, \frac{1}{2}$

tail coordinates, $(1, -1, 0)$ Miller indices = $[\bar{1}41]$

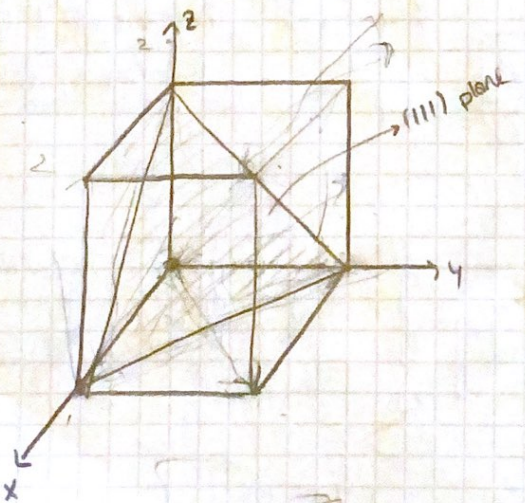
For (2), head coordinates, $(1,1,1)$ head - tail = $1, 1, 2$

tail coordinates; $(0,0,-1)$ Miller indices = $[112]$

For (3); head coordinates; $(1,-1,1)$ head - tail = $1, -2, 0$

tail coordinates; $(0,1,1)$ Miller indices = $[1\bar{2}0]$

Q5)



a, c & d

Q6) $T = 973\ K$

$Q_v = 1.28 \times 10^{-19}\ J/atom = 0.8\ eV/atom$

$\rho = 9.35\ g/cm^3$

$A = 107.9\ g/mol$

$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)$$

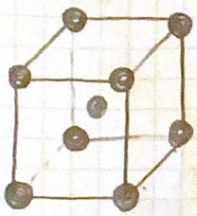
For $1m^3$, $N = \rho \times \frac{N_A}{A} \times 1m^3 = 9.35\frac{g}{mol} \times \frac{6.02\times10^{23}}{107.9} \times 1m^3 = 5.2 \times 10^{28}$

$$N_v = \underbrace{e^{\left(\frac{-0.8}{8.62\times10^{-5}\times1273}\right)}}_{6.82\times10^{-4}} \times 5.2\times10^{28} = 3.5\times10^{25} \text{ vacancies}$$

Q7) ⓐ Diameter of an interstitial impurity must be substantially smaller than that of the host atoms.

Fe's radius = 0.124 nm

And has a BCC structure.



The atom which will get into the blank spaces must have a smaller radii than Fe.

Therefore,

C = 0.071, H = 0.046, and O = 0.060 can form interstitial solid solution with Fe.

ⓑ To be soluable; 1) $\Delta r < 15\%$
2) crystal structures should be same
3) electronegativities should be comparable
4) solute's valency > solvent's valency

Cr's radius; 0.124 nm

$\left(\frac{\text{Cr's radius} - \text{Fe's radius}}{\text{Cr's radius}}\right) \times 100 < 15$; First rule ✓

Both have BCC structure, Second rule ✓

Electronegativities are close ; Third rule ✓

Solvent is Cr ; Forth rule ✓

Fe form substitutional solid solution with complete solubility with Cr.

© To form a partial soluble solution, three of Hume-Rothery rule must apply.

→ Co
- $\Delta r < 15\%$
- Structure
- Electronegativity
- Valency

First rule ✓
Second rule ×
Third rule ✓
Fourth rule ✓
} Three rules apply

→ Ag;
- $\Delta r = 16\%$
- Structure
- Electronegativities
- Valencies

First rule ×
Second rule ✓
Third rule ✓
Fourth rule ✓
} Three rules apply.

→ Al,
- $\Delta r = 15\%$
- Structure ✓
- Electronegativities
- Valencies

First rule ×
Second rule ✓
Third rule ✓
Fourth rule ✓
} Three rules apply

→ Cr,
- $\Delta r < 15\%$
- Structure ×
- Electronegativities
- Valencies

First rule ✓
Second rule ×
Third rule ✓
Fourth rule ✓
} Three rules apply

→ Fe,
- $\Delta r < 15\%$
- Structure
- Electronegativities
- Valencies

First ✓
Second ×
Third ✓
Fourth ✓
} Three rules apply

→ Zn;
- $\Delta r < 15\%$
- Structure
- Electronegativities
- Valencies

First ✓
Second ×
Third ✓
Fourth ✓
} Three rules apply

Co, Ag, Al, Cr, Fe and Zn forms substitutional solid solution with partial solubility with Ni.

Q8)

a) $E = \frac{\sigma}{\epsilon}$ → stress, → strain

before plastic deformation started; $E = \frac{\sigma}{\epsilon} = \frac{42\,MPa}{0.01} = 4.2\,GPa$

b) We draw line with slope of 4.2 GPa from 0.002 strain. We call 0.2% offset strength where this line intercepts with our Egineering stress-strain curve.

By approximation; steel yield strength = 54 MPa

c) 86 MPa

d) $U_r = \frac{1}{2}\sigma_y \epsilon_y = \frac{\sigma_y^2}{2E} = 0.3471\ MPa$

e) Total Area under Curve = 27 MPa

Q9)

(b) proportionality limit shown as a dot on the graph.

$\epsilon = 0.215$

Lower yield point ⇒ 0.000212

tensile strength ⇒ 0.000355

fracture stress ⇒ 0.00024

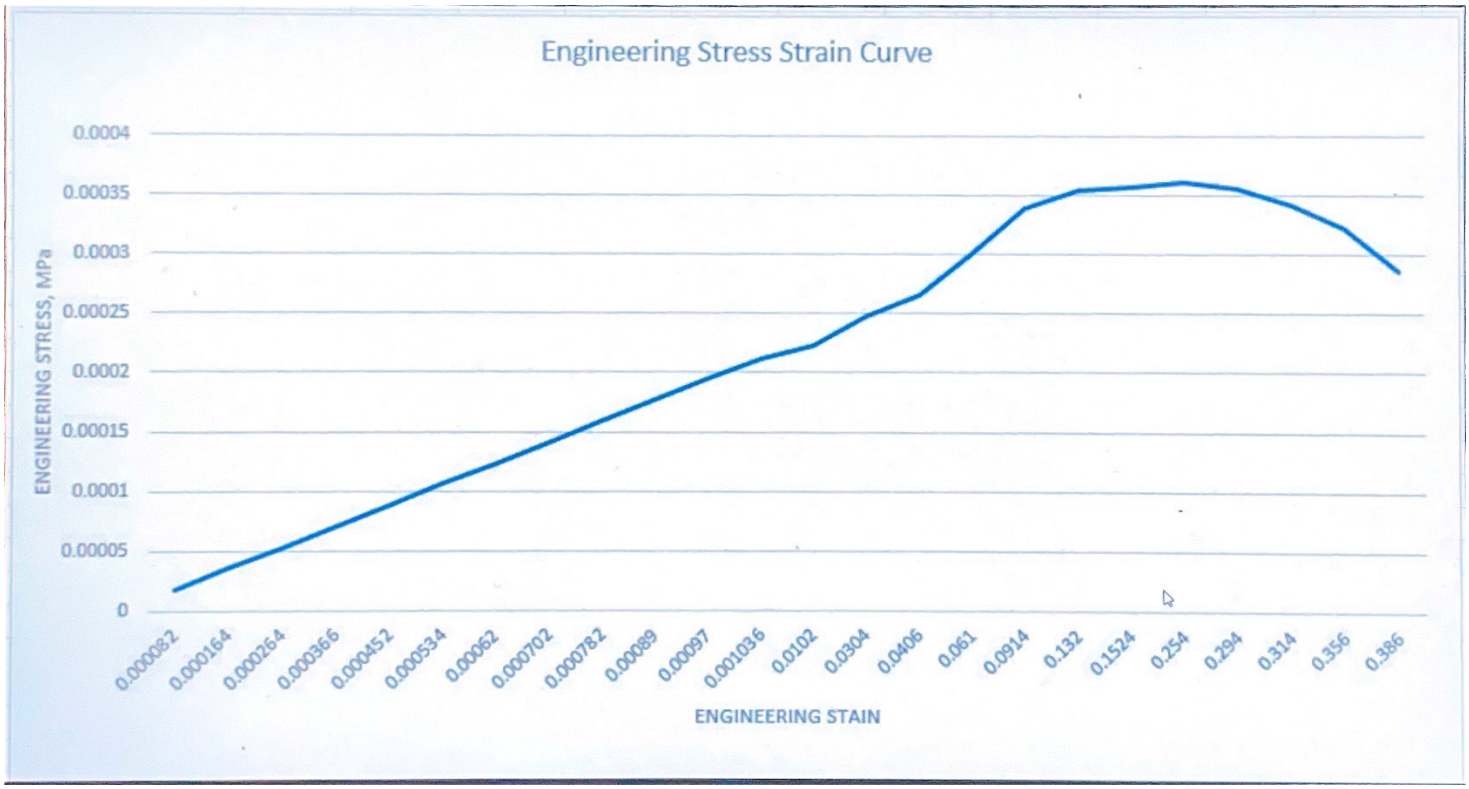
percentage elongation ⇒ 45.6 %.

reduction of area ⇒ 72.4375

Q10)

a - steel file ; 6.5
b - chalk ; 3
c - pine plank ; 2
d - ball bearing ; 6
e - sapphire ; 9

9a


Engineering Stress Strain Curve
ENGINEERING STRESS, MPa
0.0004
0.00035
0.0003
0.00025
0.0002
0.00015
0.0001
0.00005
0
0.000082
0.000164
0.000264
0.000366
0.000452
0.000534
0.00062
0.000702
0.000782
0.00089
0.00097
0.001036
0.0102
0.0304
0.0406
0.061
0.0914
0.132
0.1524
0.254
0.294
0.314
0.356
0.386
ENGINEERING STAIN