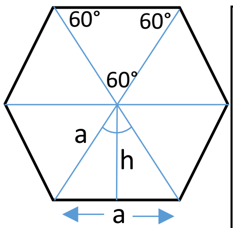
Test 1: EGR 235: Engineering Materials & Composites

10/14/2020

Answer any 4 question to get full credit (60). Answer all to get bonus credit (30)

1. (a) Derive the expression for a unit cell volume of Hexagonal Close-Packed (HCP) crystal structure.



Volume of HCP unit cell = area of hexagonal face x height of hexagonal prism

Area of hexagonal face = area of each triangle x 6

Area of triangle = ½ x base x height

= ½ x a x h

Cos 30° = h/a ⟹ h = a Cos 30° ⟹ h = $a\sqrt{\frac{3}{2}}$

= (½)$(a)(a\sqrt{\frac{3}{2}})$

= $\frac{a^2\sqrt{3}}{4}$

Area of hexagonal face = 6 $(\frac{a^2\sqrt{3}}{4})$

Volume of HCP = 6 $(\frac{a^2\sqrt{3}}{4})$

(b). Berilum (Be) has an HCP unit cell for which the ratio of the lattice parameters c/a is 1.568. If the radius of Be atom is 0.1143 nm. (a) Determine the unit cell volume and (c) Calculate the theoretical density of Be.

$v_{c=6R^2c\sqrt{3}}$

$c = 1.568(2R) = 3.13R$

$v_{c=6(3.13)R^3\sqrt{3}}$

$v_{c=6(3.13)(0.11\times10^{-7})^3\sqrt{3}}$

$v_{c=4.3\times10^{-23}cm^3\ \ per\ unit\ cell}$

$$\rho = \frac{nA}{v_cN} = \frac{6(9.01)}{(4.3\times10^{-23})(6.022\times10^{23})} = 2.07g/cm^3$$

2. Iron (Fe) undergoes an allotropic transformation at high temperature from a BCC to FCC. An atomic radius R_{BCC}=0.12584 nm transforms to R_{FCC}=0.12894 nm. Compute the percentage volume change associated with this transformation. Does the volume increase or decrease? (15)

BCC = 2 atoms

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

$$a = \frac{4 \times 0.12584}{\sqrt{3}}$$

$$a = 0.29062$$

$$\frac{volume}{atom} = \frac{a^3}{2}$$

$$\frac{volume}{atom} = \frac{0.29062^3}{2}$$

$$\frac{volume}{atom} = 0.01227$$

FCC = 4 atoms

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

$$a = \frac{4 \times 0.12894}{\sqrt{2}}$$

$$a = 0.36470$$

$$\frac{volume}{atom} = \frac{a^3}{4}$$

$$\frac{volume}{atom} = \frac{0.36470^3}{4}$$

$$\frac{volume}{atom} = 0.01213$$

$$\frac{Change\ in\ volume}{Original\ volume} \times 100 = \frac{0.01227 - 0.01213}{0.01227} \times 100 = 1.14\%$$

3. Calculate the density of the material given that its atomic weight is 141 g/mol with BCC crystal structure and lattice parameter of 0.35 nm. (15)

$$\rho = \frac{nA}{v_c N} = \frac{2(141)}{(3.5\times10^{-23})(6.022\times10^{23})} = 13.38 g/cm^3$$

4. Compare the Atomic packing Factors of SCC, FCC and BCC crystal structures (15)

SCC - has 1 unit cell per atom. The side of the unit cell is of length 2*r*, where *r* is the radius of the atom.

$$APF = \frac{N_{atoms} V_{atoms}}{V_{unit\ cell}} = \frac{1\times\frac{4}{3}\pi r^3}{(2r)^3} = \frac{\pi}{6} \approx 0.52\ or\ 52\%$$

BCC – has 2 unit cell per atom. The side of the unit cell is the length of 4*r* /√3

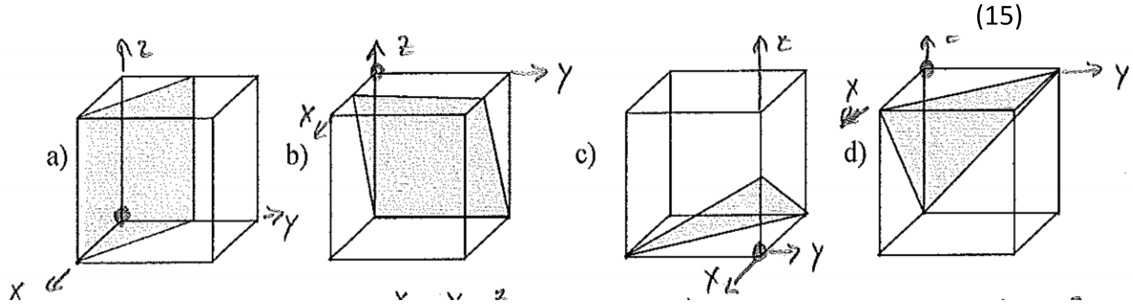
$$APF = \frac{N_{atoms}V_{atoms}}{V_{unit\ cell}} = \frac{2\times\frac{4}{3}\pi r^3}{(\frac{4r}{\sqrt{3}})^3} = \frac{\pi\sqrt{3}}{8} \approx 0.68\ or\ 68\%$$

FCC – has 4 unit cell per atom. The side of the unit cell is of length 4r /$\sqrt{2}a$

$$APF = \frac{N_{atoms}V_{atoms}}{V_{unit\ cell}} = \frac{4\times\frac{4}{3}\pi r^3}{(2\sqrt{2}r)^3} = \frac{\pi\sqrt{2}}{6} \approx 0.74\ or\ 74\%$$

5. Determine miller indices for the following planes (be sure to redraw the cubes and identify the axis)

(15)



6. Determine the plane with highest plannar density in the following crystal structure

(15)

(a) BCC
(b) FCC