HW 3

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E45

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Problem 3.70. The diffraction peaks labeled in Figure 3.33 correspond to the reflection rules for an FCC metal (h, k, l unmixed, as shown in Table 3.4). What would be the hkl indices for the three lowest diffraction-angle peaks for a bcc metal?

The rule for bcc metals state that $h + k + l =$ even number. Also the indices start from the lowest possible combination and work up. Using these simple rules we can find the first 3 peaks.

Peak	hkl indices	proof of even number
1	(110)	$1 + 1 + 0 = 2$
2	(200)	$2 + 0 + 0 = 2$
3	(211)	$2 + 1 + 1 = 4$

Problem 3.80. Calculate the first six diffraction peak positions for MgO powder using CuK_α radiation. (This ceramic structure based on the fcc lattice shares the reflection rules of the fcc metals).

The edge length a of a fcc bravais lattice with two ions is $a = 2(r_{\text{anion}} + r_{\text{cation}})$. So the edge length for MgO is $a = 0.420$nm and $\lambda_{\text{CuK}_\alpha} = 0.1542$nm. Using this we can solve the Bragg's equation for the simple case of n = 1,

$$\theta = \arcsin \frac{\lambda}{2d} \tag{1}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{2}$$

Peak	hkl indices	d_{hkl} (nm)	2θ (degrees)
1	(111)	0.242	37.1
2	(200)	0.210	43.1
3	(220)	0.148	62.6
4	(311)	0.127	75.0
5	(222)	0.121	79.0
6	(400)	0.105	94.5

Problem 4.19. Calculate the density of Schottky pairs (in m^{-3}) in MgO if the fraction of vacant lattice sites is 5×10^{-6}. (The density of MgO is 3.60 Mg/m^3).

$$\text{atom density} = \frac{\rho}{\text{atom mass}} = \frac{3.60 \times 10^6 g/m^3}{(24.31 + 16.00)g/(6.02 \times 10^{23}\text{atoms})} = 5.376 \times 10^{28}\,\text{atoms}/m^3$$

$$\text{vacancy density} = 5 \times 10^{-6}\text{atoms}^{-1} \times 5.376 \times 10^{28}\text{atoms} * m^{-3} = 2.69 \times 10^{23} m^{-3}$$

Problem 4.21. The energy necessary to generate a dislocation is proportional to the square of the length of the Burgers vector, $|b|^2$. This relationship means that the most stable (lowest energy) dislocations have the minimum length, $|b|$. For the bcc metal structure, calculate (relative to $E_{b=[111]}$) the dislocation energies for **(a)** $E_{b=[110]}$ and **(b)** $E_{b=[100]}$.

Since $E \propto |b|^2$, we can compare ratios relative to $|b|_{[111]}$. Also the edge length of a bcc is a and the diagonal across the base is $\sqrt{2}a$. Note for a bcc, $a = 4R/\sqrt{3}$.

(a)

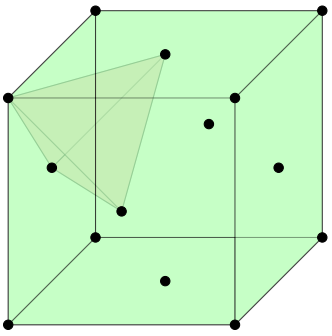
$$\frac{E_{b=[110]}}{E_{b=[111]}} = (\frac{|b_{[110]}|}{|b_{[111]|}})^2 = (\frac{\sqrt{2}a}{2R})^2 = (\frac{\sqrt{2}4R/\sqrt{3}}{2R})^2 = \frac{8}{3} = 2.67$$

(b)

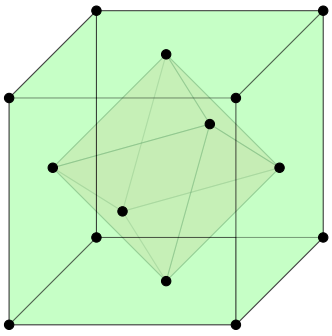
$$\frac{E_{b=[100]}}{E_{b=[111]}} = (\frac{|b_{[100]}|}{|b_{[111]|}})^2 = (\frac{a}{2R})^2 = (\frac{4R/\sqrt{3}}{2R})^2 = \frac{4}{3} = 1.33$$

Problem 4.30. As Figure 4.20 shows, noncrystalline metal has a range of space-filling polyhedra comprising its structure. Similarly, the FCC structure can be represented by a repetitive polyhedra structure, which is an alternative to our usual unit cell configuration. In other words, the fcc structure can be equally represented by a space-filling stacking of regular polyhedra (tetrahedra and octahedra in a ration of 2:1). (a) Sketch a typical tetrahedron (four-sided figure) on a perspective sketch such as Figure 3.5(a). (b) Similarly, show a typical octahedron (eight-sided figure). Note also Problem 3.60.)

Drawn in latex using tikz package



(a)



(b)