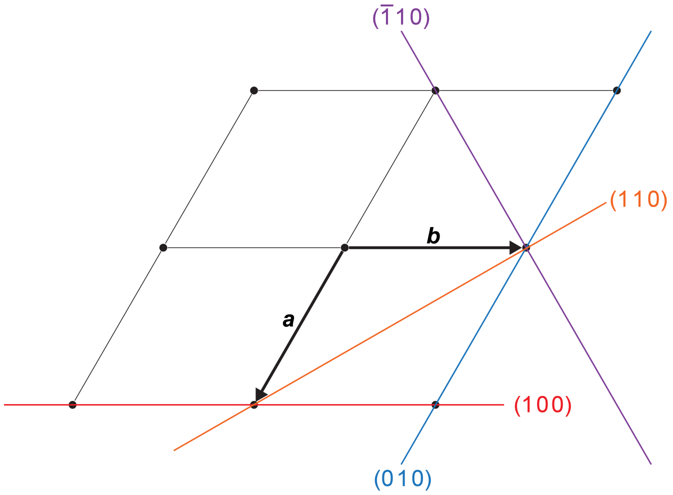
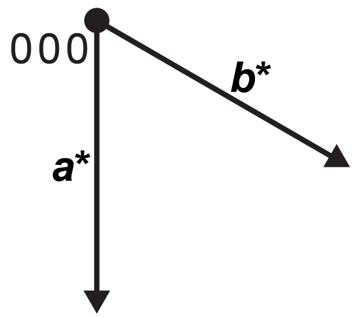
Assignment Week 3 – Answers

Assignment 3.1

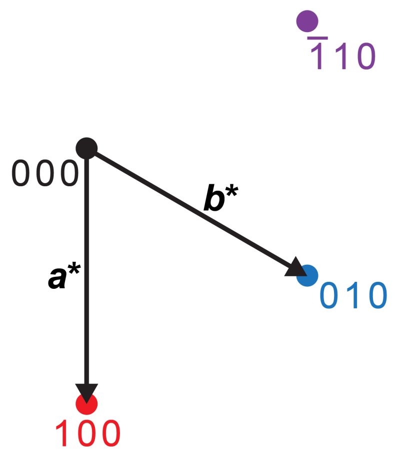
a) Each trace for plane $(h\ k\ 0)$ intersects the X-axis at distance a/h from the origin and the Y-axis at distance b/k from the origin. Therefore, the plane traces should look as shown here. (Note if multiple parallel traces per plane $(h\ k\ 0)$ are shown the answer is still valid, as long as the plane traces are separated by the correct distances.)



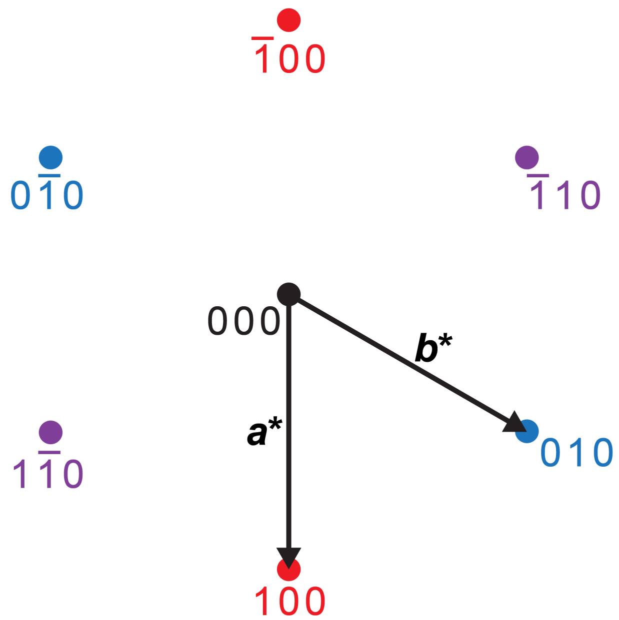
b) i) The reciprocal lattice vectors ***a**** and ***b**** should have the same length, and should be drawn perpendicular to the traces of the (1 0 0) and (0 1 0) planes from part (a), like this:



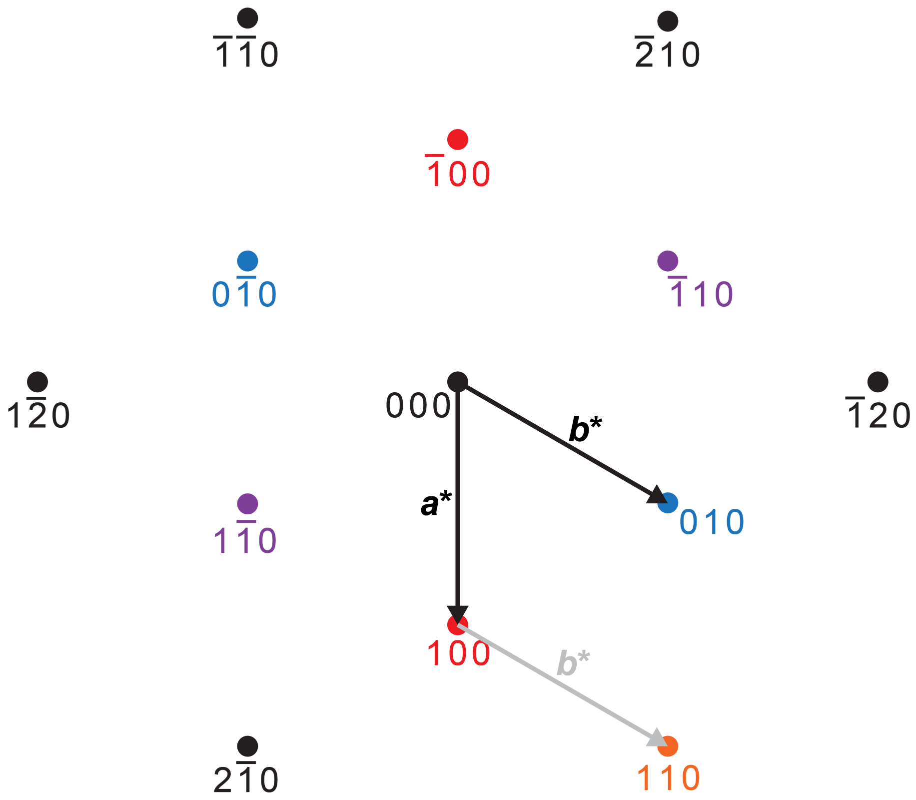
ii) The reciprocal lattice nodes for the (1 0 0) and (0 1 0) planes should be placed at the ends of the vectors ***a**** and ***b**** respectively. The $(\bar{1}\ 1\ 0)$ node should be at the same distance from the origin, but should be perpendicular to the $(\bar{1}\ 1\ 0)$ plane trace drawn earlier:



iii) The inverse of the (1 0 0), (0 1 0) and $(\bar{1}\ 1\ 0)$ planes are the $(\bar{1}\ 0\ 0)$, $(1\ \bar{1}\ 0)$ and $(1\ \bar{1}\ 0)$ planes. Relative to the origin their nodes should be drawn at the inverse locations of the previously drawn planes:



iv) The reciprocal lattice node for the (1 1 0) plane can be found by vectorial addition of ***a**** and ***b****, i.e.: 1 0 0 + 0 1 0 = 1 1 0. Similarly, the node for $\bar{2}$ 1 0 = $\bar{1}$ 1 0 + $\bar{1}$ 0 0 and the node for $\bar{1}$ 2 0 = $\bar{1}$ 1 0 + 0 1 0. Their inverse counterparts are done as before. The final diagram should look like the one below. *Note that the node for the (1 1 0) plane is perpendicular to its plane trace drawn previously, as is correct.*



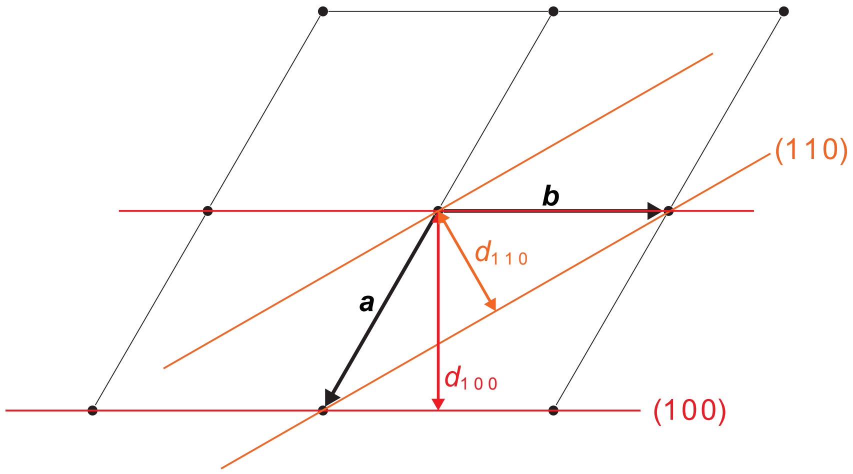
v) The reciprocal lattice nodes have a 6-fold or hexad rotational symmetry, the same as that of the crystal lattice in this [0 0 1] orientation.

Assignment 3.2

a) To answer part a), first the plane spacings must be calculated. Do the plane spacings match those described below? Answers should be correct to at least 2 significant figures.

The plane spacing $d_{h\,k\,l}$ is the perpendicular distance between the $(h\;k\;l)$ planes. From the diagram below for a hexagonal lattice, it is evident that:

$$d_{1\,0\,0} = a\cos(60°) = a\frac{\sqrt{3}}{2} \qquad d_{11\,0} = \frac{a}{2} \qquad \text{Further: } d_{2\,0\,0} = \frac{d_{1\,0\,0}}{2} = a\frac{\sqrt{3}}{4}$$



Using a = 0.3209 nm the following plane spacings are therefore obtained:

$h\,k\,l$	$d_{h\,k\,l}$ (nm)
1 0 0	0.2779
1 1 0	0.1605
2 0 0	0.1390

Second the scattering angle must be calculated from the plane spacings. Do the values match those described below? Answers should be correct to at least 2 significant figures.

The scattering angle measured in TEM is $2\theta_B$. Using the small angle approximation of the Bragg equation we find:

$$\lambda = 2d_{h\,k\,l}\sin\theta_B \approx 2d_{h\,k\,l}\theta_B \quad \text{Rearranging: } 2\theta_B \approx \frac{\lambda}{d_{h\,k\,l}}$$

Using the previously calculated plane spacings, for λ = 1.97 pm the scattering angles are:

$h\,k\,l$	$2\theta_B$ (mrad)
1 0 0	7.09
1 1 0	12.28
2 0 0	14.17–14.18

b) When acceleration voltage is decreased, the scattering angle increases. This is because, as the energy of the electron beam decreases, its wavelength increases, and the scattering angle increases in proportion with the wavelength. For example, for a 200 keV beam with $\lambda = 2.51$ pm, for the (1 0 0) plane $2\theta_B = 9.03$ mrad.

c) Although the (1 0 0) and (2 0 0) planes are parallel, the reciprocal lattice node for the (2 0 0) plane is two times further from the (0 0 0) origin than that of the (1 0 0) plane. Therefore, if the Ewald sphere cuts the (1 0 0) node exactly, it cannot cut the (2 0 0) node (and vice versa), as shown in the diagram below.