# Condensed matter physics 2013
# Solutions for Exercise 3

Release: 8. Oct. 2013

## Problem 11 (2p)

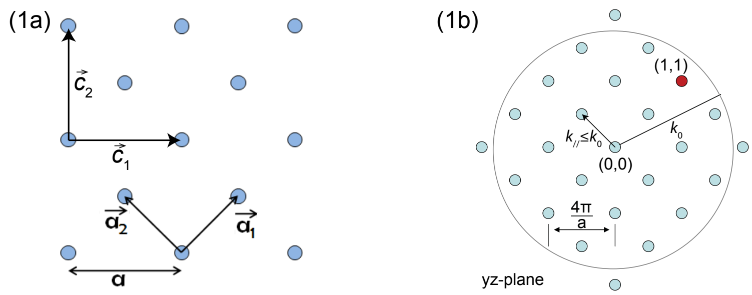
Given in the problem: kinetic energy $E = 150\,\text{eV}$ and lattice spacing $a = 3.89\text{Å}$.

a) Radius of Ewald sphere:

$$E = \frac{\hbar^2 k_0^2}{2m} \Rightarrow k_0 = 6.27\cdot 10^{10}\,\text{m}^{-1} = 24.4\cdot \frac{1}{a}$$

b) Direct (real space) lattice of Pd at the (1,0,0) surface (fcc)

It is custom to use the orthogonal cubic basis vectors ($\vec{c}_1, \vec{c}_2$ in figure 1a) and not the primitive ones ($\vec{a}_1, \vec{a}_2$). The latter are used to construct the reciprocal lattice.




c) The corresponding reciprocal lattice:

Because the penetration depth of the electrons is small, i.e. one atomic layer, we only consider one lattice plane. This breaks the translation symmetry perpendicular to the (1,0,0) plane. Since this layer is very small the allowed $k$-states along $x$ lie very close and form a continuum (see script page 2.13). Each blue point in figure 1b represents a rod, perpendicular to the page. All points on these rods form the reciprocal 'lattice'.

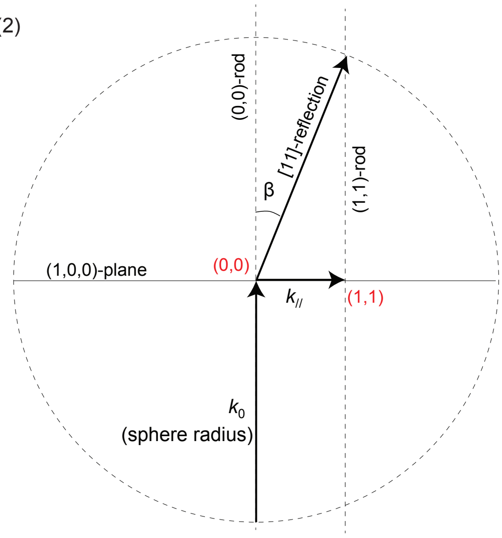
d) Construction of Ewald's sphere (in units of $\frac{1}{a}$)

The incident $\vec{k}_0$ lies on the rod through the reciprocal lattice site (0,0) in the (1,0,0) plane and ends on (1,1) (the starting point needs to lie on a point of the reciprocal lattice). The Ewald sphere is a sphere with radius $k_0$ around (0,0,0) (by definition). Where this sphere intersects the rods, a reflection is allowed (elastic scattering $\rightarrow$ amplitude of k-vector is the same for the incident and for the scattered electron). In the figure below each point in the 'Ewald circle' represents a rod that intersects the Ewald sphere. (The projection of the scattered $k$-vector onto the $yz$-plane has to be smaller than $k_0$). In total there are 21 reflexes allowed (points inside the circle).

e) Calculation of the scattering angle of the [11]-reflection (red point in figure 1b):

Figure 2 shows a cross section of the Ewald sphere in the plane containing the vector (1,1) and $\vec{k}_0$. The rod through (1,1) is depicted as dashed line parallel to $\vec{k}_0$ and the scattered electron $k$-vector is denoted as '[1,1]-reflection' (same amplitude as $\vec{k}_0$). The projection onto the reciprocal yz-plane is $\vec{k}_{\|}$, pointing from (0,0) to the (1,1). Then we find

(2)




$$k_{\parallel} = \left|\vec{k}_{\parallel}\right| = \frac{4\pi}{a}\left|\begin{pmatrix}1\\1\\0\end{pmatrix}\right| = \frac{4\sqrt{2}\pi}{a}$$

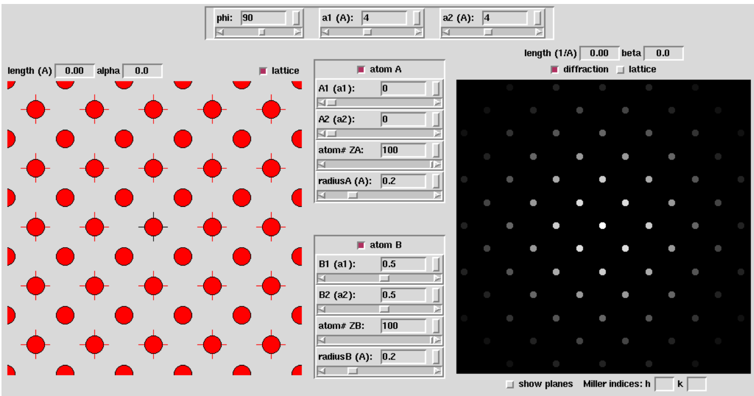
$$\sin(\beta) = \frac{k_{\parallel}}{k_0} = \frac{\frac{4\sqrt{2}\pi}{a}}{24.4\frac{1}{a}} = 0.73$$

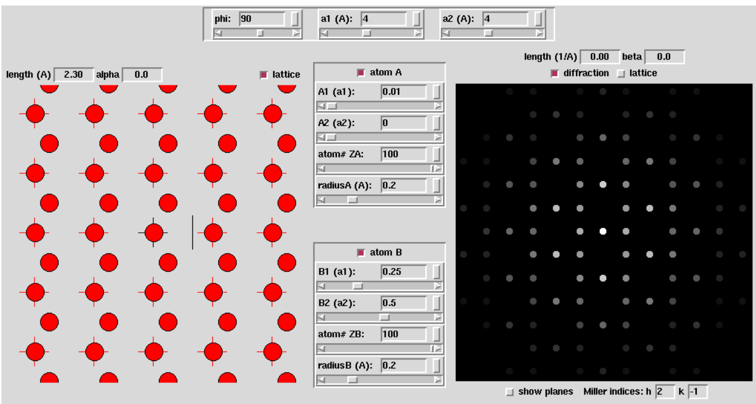
$$\Rightarrow \beta = 46.7^{\circ}$$

## Problem 12

a) Its reciprocal lattice keeps the $C_4$ symmetry, but those indices with a mixture of odd and even will disappear (destructive interference) – see fig. **a)**

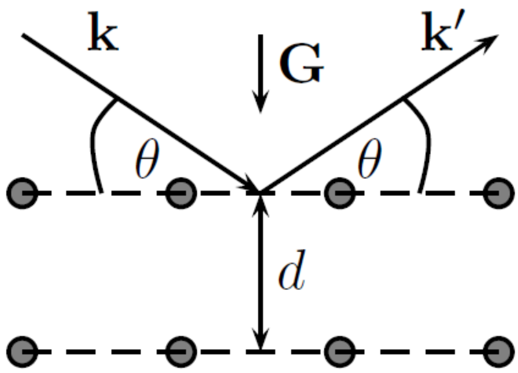
b) see figure **b)**





## Problem 13 ((a):1p, (b):3p)

**a)** Consider the following picture. Here we have shown the reciprocal lattice vector $\vec{G}$ which corresponds to the family of lattice planes. As we discussed in previous, the spacing between lattice planes is $d = 2\pi/|\vec{G}|$.




Just from geometry we have

$$\vec{k} \cdot \vec{G} = sin\theta = -\vec{k'} \cdot \vec{G}$$

Suppose the Laue condition is satisfied. That is, $\vec{k} - \vec{k'} = \vec{G}$ with $|\vec{k}| = |\vec{k'}| = 2\pi/\lambda$. We can rewrite the Laue equation as

$$\frac{2\pi}{\lambda}(\vec{k} - \vec{k'}) = \vec{G}$$

Now let us dot this equation with $\vec{G}$ to give

$$\vec{G} \cdot \frac{2\pi}{\lambda}(\vec{k} - \vec{k'}) = \vec{G} \cdot \vec{G}$$

$$\frac{2\pi}{\lambda}(sin\theta - sin\theta') = |\vec{G}|$$

$$\frac{2\pi}{|\vec{G}|}(2sin\theta) = \lambda$$

$$2sin\theta = \lambda$$

**b)** The distance between planes with orientation $(hkl)$ is:

$$d_{hkl} = \frac{2\pi}{|\vec{q}_{hkl}|}$$

for cubic latices:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Bragg's Law:

$$n\lambda = 2d_{hkl}\sin\theta$$

It will be shown in problem 14 (appologies...) that there are no reflections for planes with only odd or only even indices, so there is no need to calculate these. This leads to

$d_{111}$ : 3.26Å
$d_{200}$ : 2.82Å
$d_{220}$ : 1.99Å
$d_{222}$ : 1.63Å
$d_{311}$ : 1.7Å
$d_{331}$ : 1.3Å
$d_{400}$ : 1.41Å
$d_{420}$ : 1.26Å
$d_{440}$ : 0.99Å

Solving for $\theta$ gives:

$\theta = 27°$: (111)
$\theta = 32°$: (200)
$\theta = 45°$: (220)
$\theta = 54°$: (311)
$\theta = 56°$: (222)
$\theta = 66°$: (400)
$\theta = 73°$: (331)
$\theta = 75°$: (420)

In case we have a NaCl single crystal with [100] out-of-plane direction, only those peaks with Miller indices (200) and (400) could be observed. Both planes are in parallel with (100) plane.