Prof. Hans Peter Büchler SS 2012, 17th of April 2012

Exercise 1 - Crystal Structure

(a) The primitive vectors for a *body center cubic* (bcc) lattice are

$$egin{array}{rcl} ec{a}_1 &=& aec{x}, \ ec{a}_2 &=& aec{y}, \ ec{a}_3 &=& rac{a}{2}(ec{x}+ec{y}+ec{z}). \end{array}$$

or, in a more symmetric set

$$\vec{a}_1 = \frac{a}{2}(-\vec{x} + \vec{y} + \vec{z}), \\ \vec{a}_2 = \frac{a}{2}(\vec{x} - \vec{y} + \vec{z}), \\ \vec{a}_3 = \frac{a}{2}(\vec{x} + \vec{y} - \vec{z}).$$

1. Make a drawing of this lattice,

2. Find the reciprocal lattice vectors and make a drawing of the reciprocal lattice.

(b) The primitive vectors for a *face center cubic* (fcc) lattice are

$$\vec{a}_1 = \frac{a}{2}(\vec{y} + \vec{z}),$$

 $\vec{a}_2 = \frac{a}{2}(\vec{x} + \vec{z}),$
 $\vec{a}_3 = \frac{a}{2}(\vec{x} + \vec{y}).$

1. Make a drawing of this lattice,

- 2. Find the reciprocal lattice vectors and make a drawing of the reciprocal lattice.
- (c) Graphically construct the Wigner-Seitz cell and the reciprocal lattice of the two dimensional oblique lattice with basis vectors $\vec{a}1$ and $\vec{a}2$ shown in the following sketch :



Exercise 2 - The Brillouin Zone

Show that the volume of the elementary cell Ω and the volume of the Brillouin Zone Ω_B are connected by the following relation :

$$\Omega_B = \frac{(2\pi)^3}{\Omega} \tag{1}$$

Exercise 3 - Tetragonal symmetry

Show that if one streches a fcc lattice along one of its lattice vectors, the resulting lattice is equivalent to a tetragonal body centered lattice. So the point group with the tetragonal symmetry has two Bravais lattices : simple tetragonal and body centered tetragonal, whereas the point group with cubic symmetry has three Bravais lattices : sc, bcc and fcc.

Exercise 4 - Fourier transformations

- 1. Calculate the Fourier coefficients for a function f(x) = c, c some number, x defined in some one-dimensional interval.
- 2. Calculate explicitly the Fourier coefficients for a function $f(x) = \exp(ip\frac{2\pi}{a}x)$, with p some integer.

Solutions due on : 20th pf April, 2012